

Chemical Profile and *In Vitro* Evaluation of the Antibacterial Activity of *Dioscorea communis* Berry Juice

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Supporting information

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1. GC-MS chromatograms of the fractions A1A, A1B, A2A, A2B, AE, AG, AI, AD_B and AF_A

1.1. GC-MS chromatograms of A1A

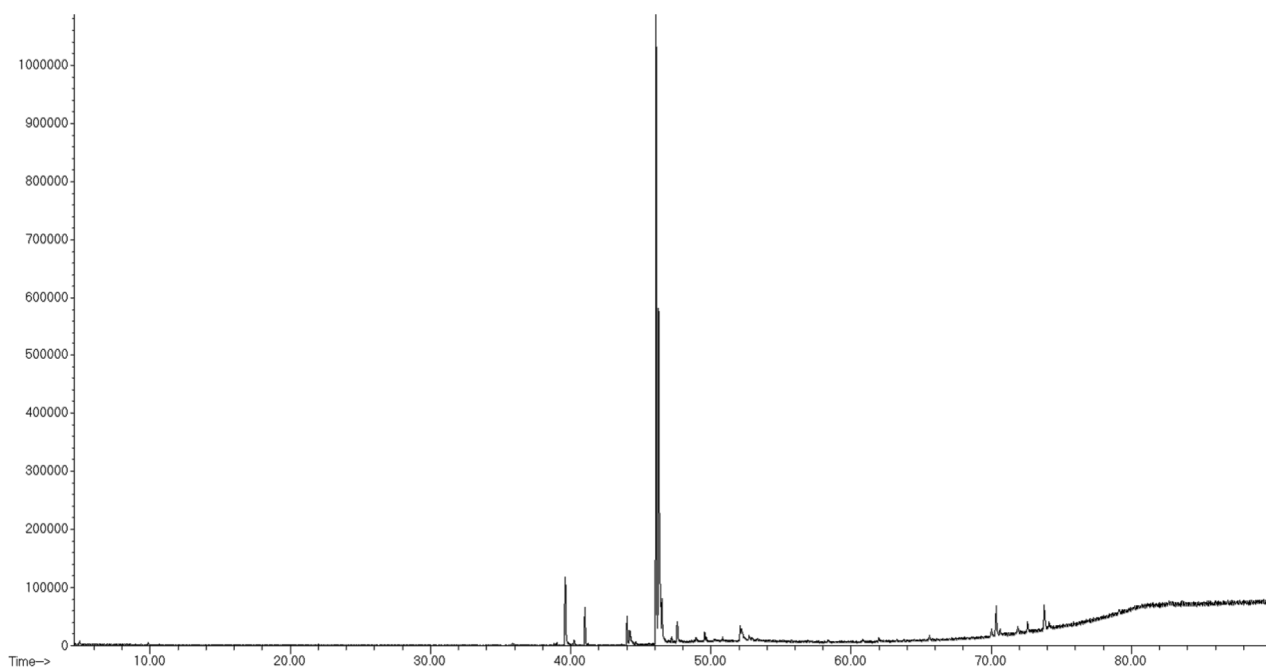


Figure S1. Total GC-MS chromatogram of A1A.

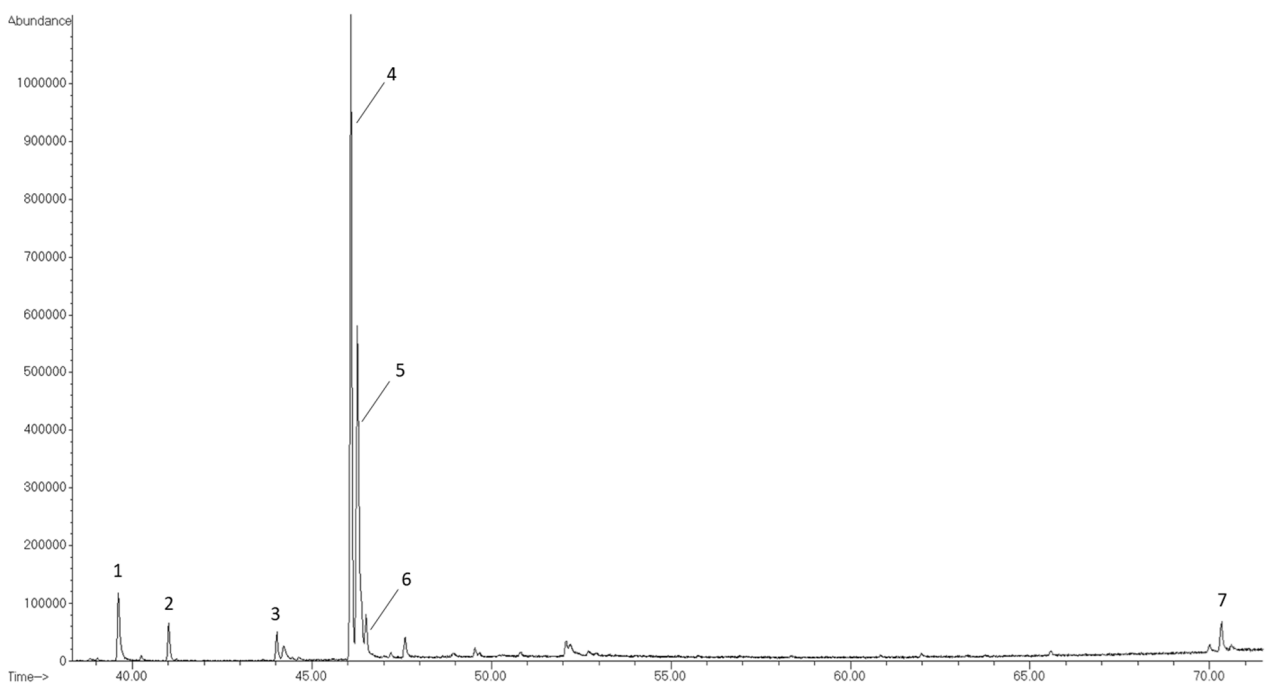


Figure S2. Zoomed GC-MS chromatogram of A1A in the region of identified compounds. 1. dibutyl phthalate, 2. ethyl palmitate, 3. methyl linoleate, 4. ethyl linoleate, 5. ethyl linolenate, 6. ethyl oleate, 7. α -tocopherol.

1.2. GC-MS chromatograms of A1B

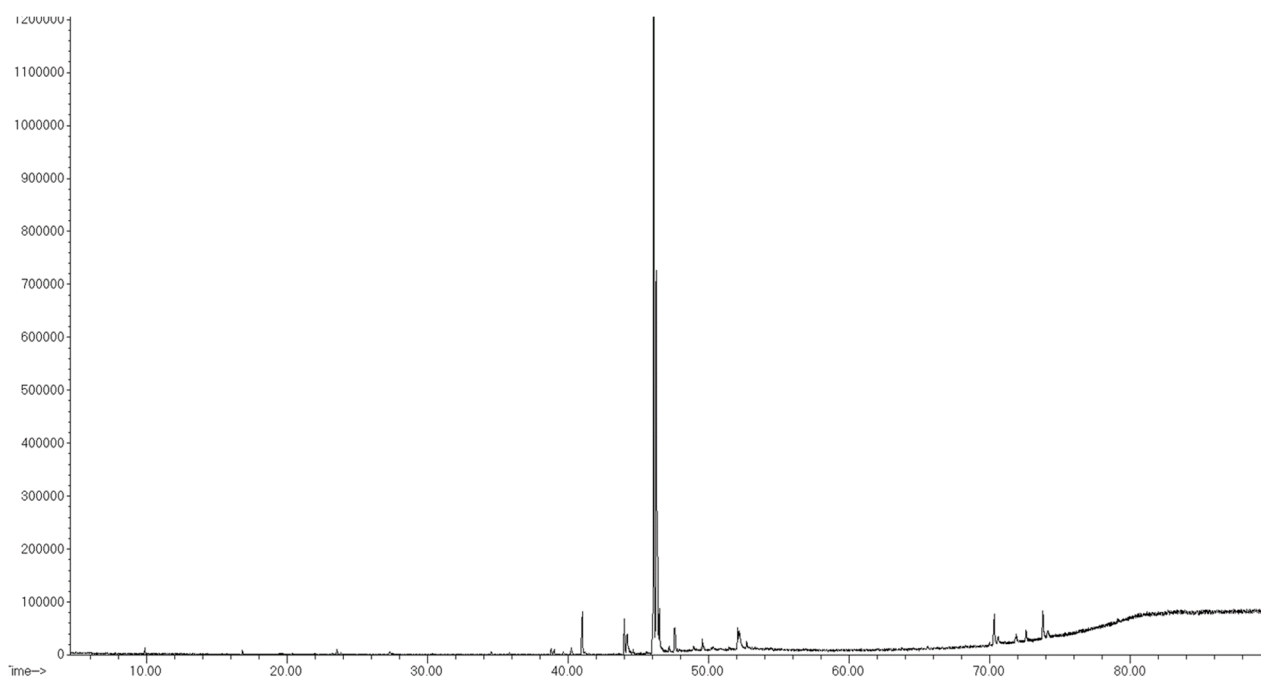


Figure S3. Total GC-MS chromatogram of A1B.

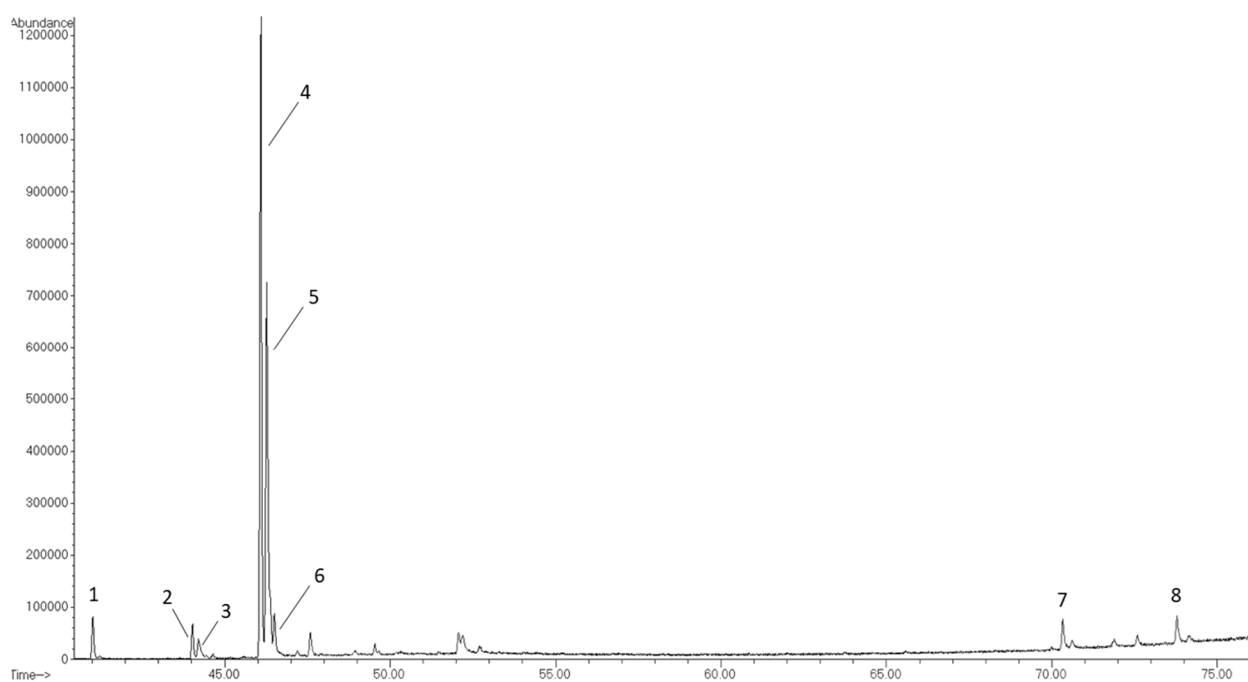


Figure S4. Zoomed GC-MS chromatogram of A1B in the region of identified compounds. 1. ethyl palmitate, 2. methyl linoleate, 3. methyl linolenate, 4. ethyl linoleate, 5. ethyl linolenate, 6. ethyl oleate, 7. α -tocopherol, 8. β -sitosterol.

1.3. GC-MS chromatograms of A2A

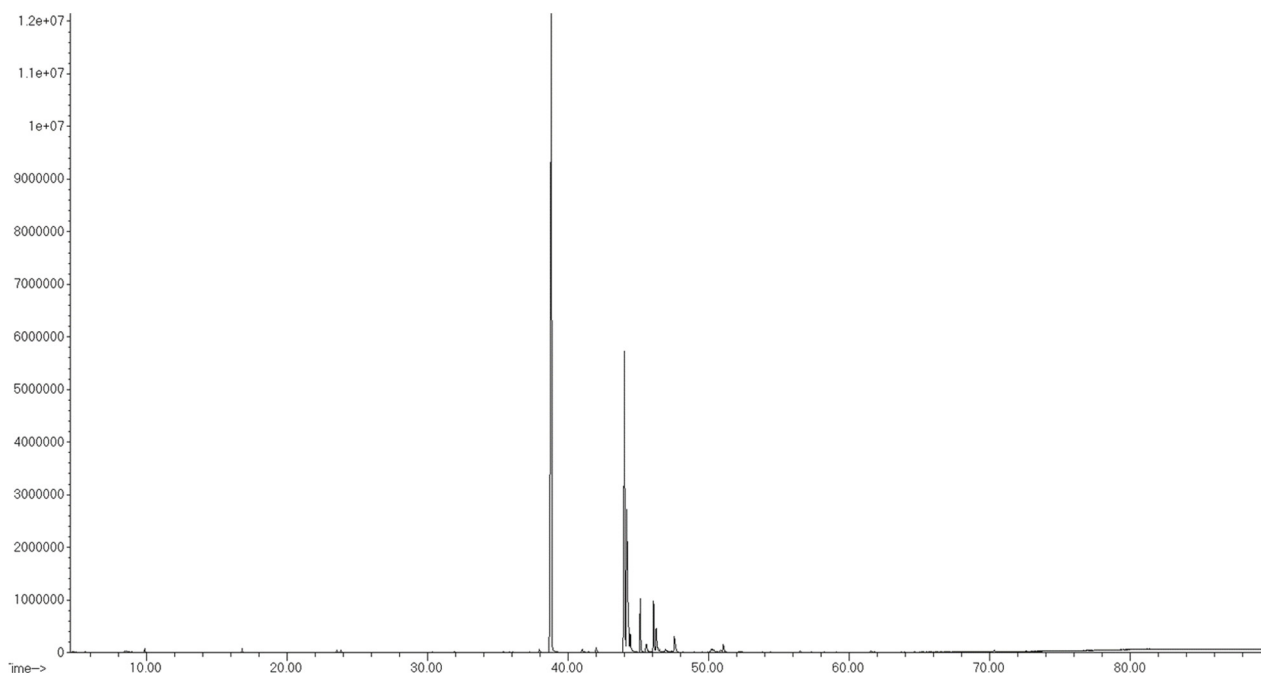


Figure S5. Total GC-MS chromatogram of A2A.

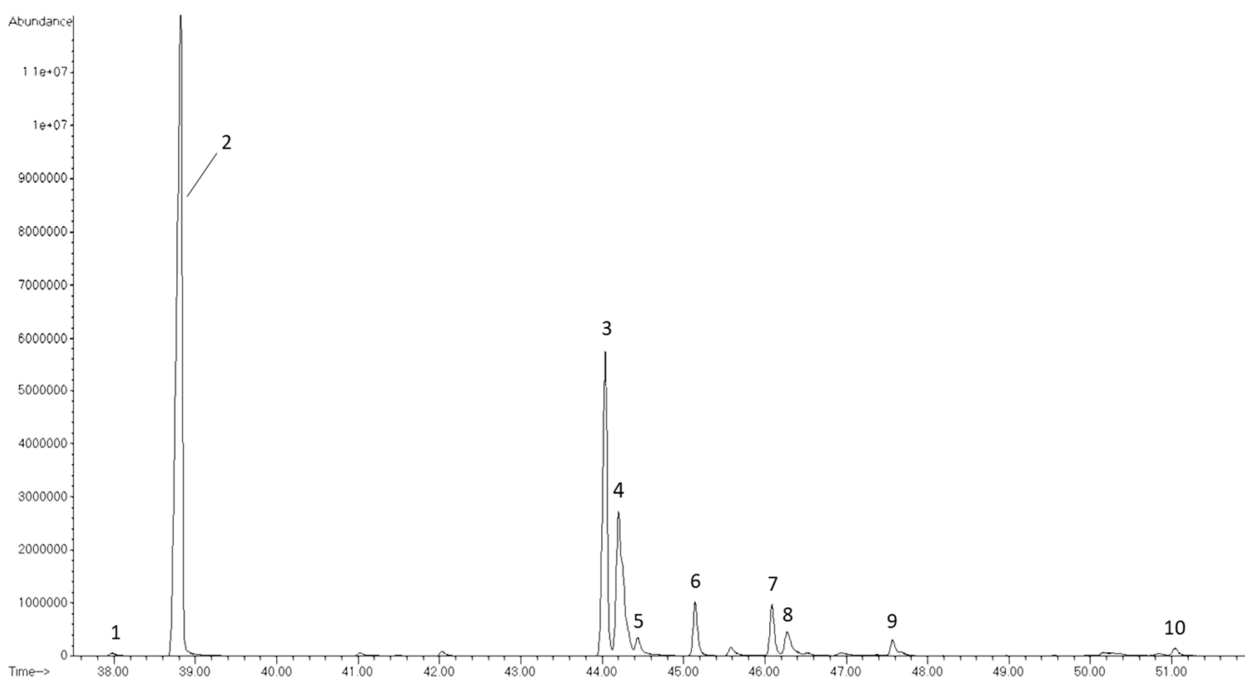


Figure S6. Zoomed GC-MS chromatogram of A2A in the region of identified compounds. 1. methyl palmitoleate, 2. methyl palmitate, 3. methyl linoleate, 4. methyl linolenate, 5. methyl oleate, 6. methyl stearate, 7. ethyl linoleate, 8. ethyl linolenate, 9. unknown [$m/z=278.3$], 10. methyl arachidate.

1.4. GC-MS chromatograms of A2B

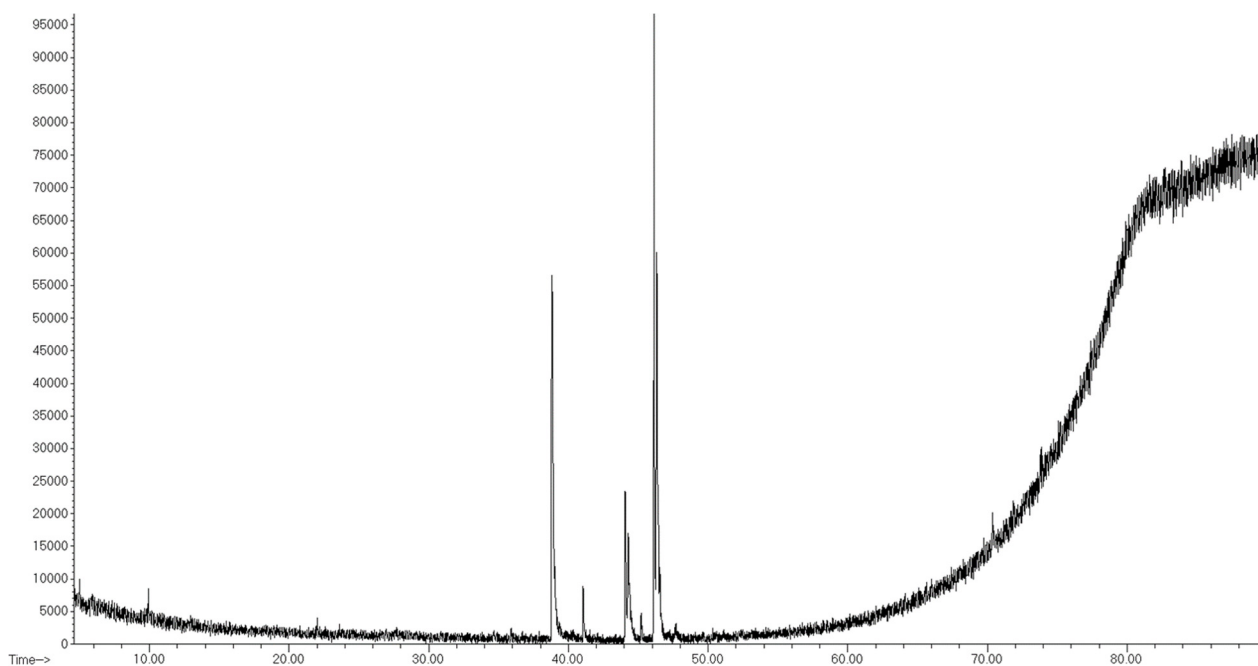


Figure S7. Total GC-MS chromatogram of A2B.

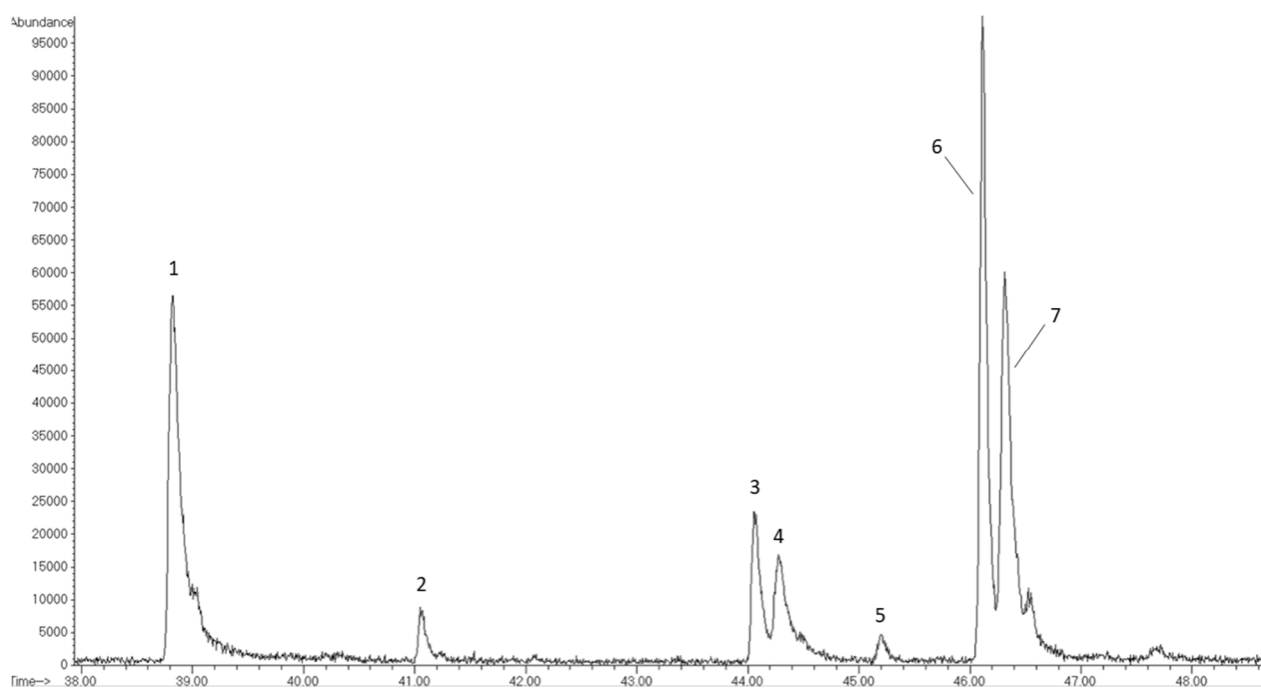


Figure S8. Zoomed GC-MS chromatogram of A2B in the region of identified compounds. 1. methyl palmitate, 2. ethyl palmitate, 3. methyl linoleate, 4. methyl linolenate, 5. methyl stearate, 6. ethyl linoleate, 7. ethyl linolenate.

1.5. GC-MS chromatograms of AE

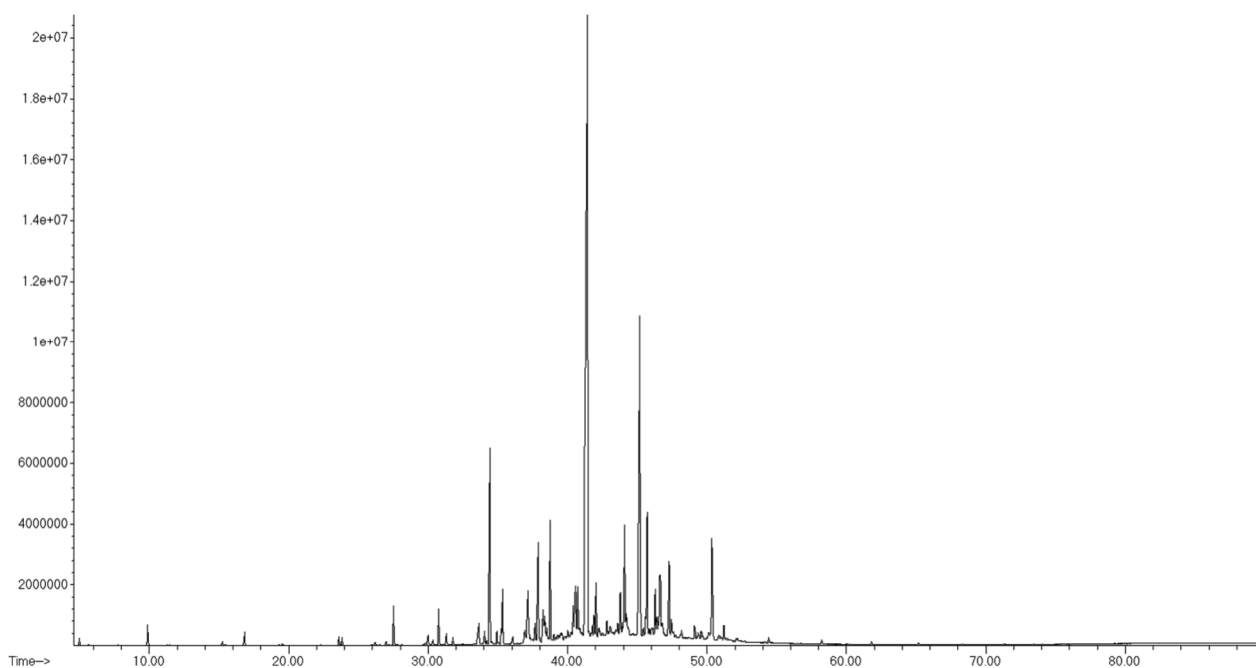


Figure S9. Total GC-MS chromatogram of AE.

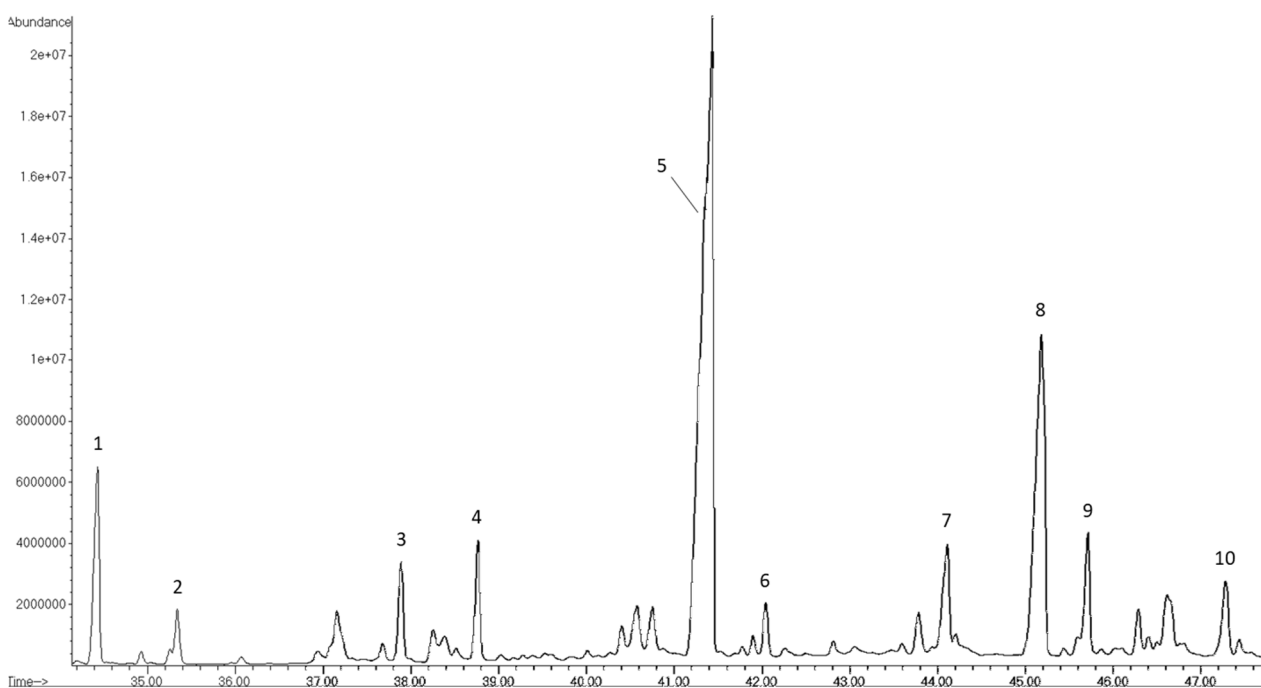


Figure S10. Zoomed GC-MS chromatogram of AE in the region of identified compounds. 1. 2-hexadecanone, 2. pentadecanoic acid, methyl ester, 3. 2-heptadecanone, 4. methyl palmitate, 5. 2-octadecanone, 6. methyl margarate, 7. methyl linoleate, 8. methyl stearate, 9. oleic acid, 10. ethyl stearate.

1.6. GC-MS chromatograms of AG

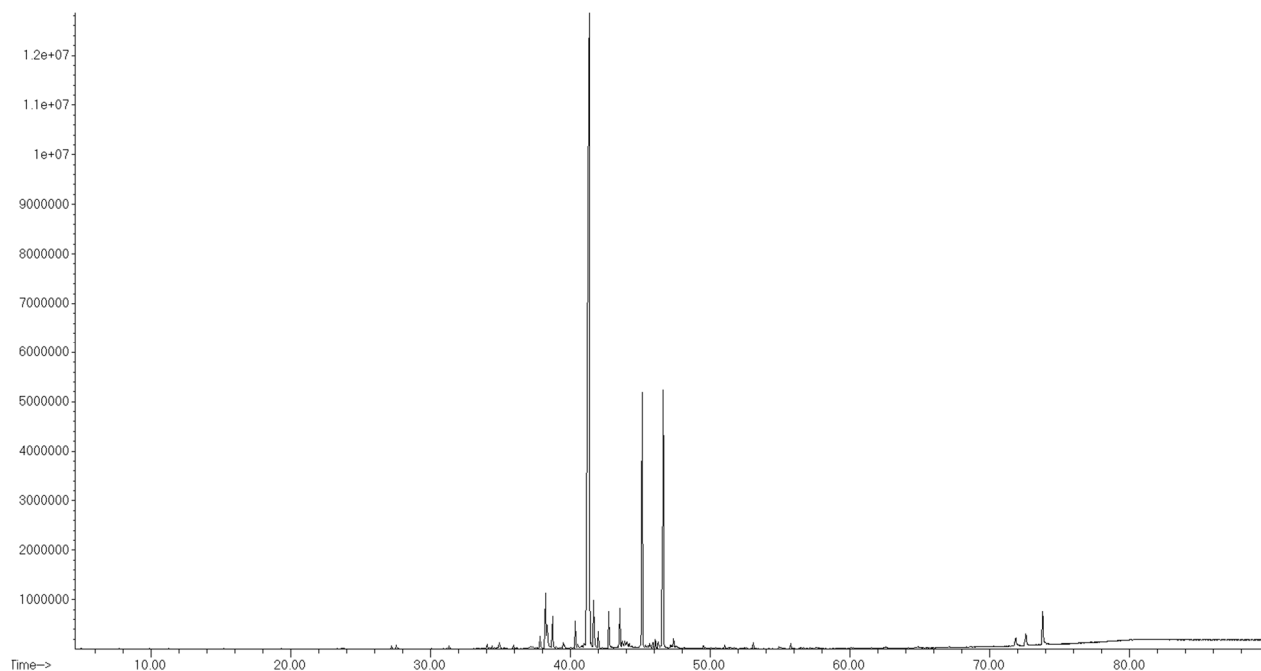


Figure S11. Total GC-MS chromatogram of AG.

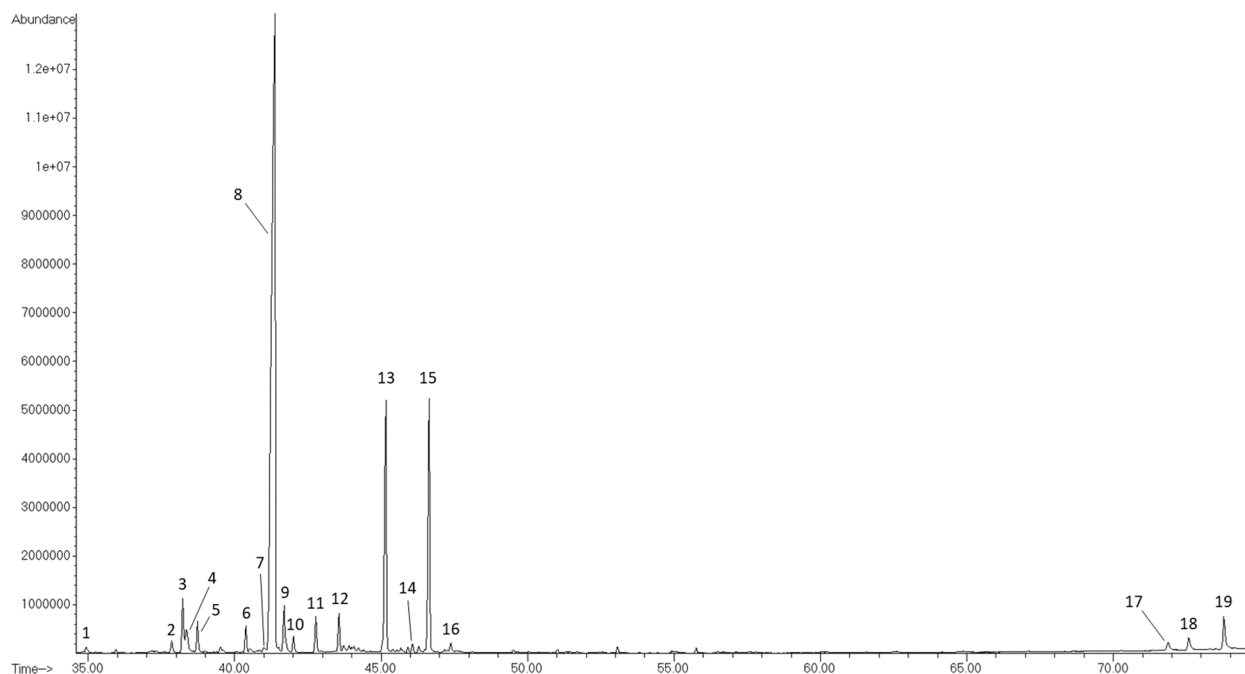


Figure S12. Zoomed GC-MS chromatogram of AG in the region of identified compounds. 1. palmitaldehyde, 2. 2-heptadecanone, 3. trans-2-nonadecene, 4. unknown [$m/z=266.1$], 5. methyl palmitate, 6. unknown [$m/z=285.1$], 7. ethyl palmitate, 8. 2-octadecanone, 9. stearaldehyde, 10. methyl margarate, 11. unknown [$m/z=282.1$], 12. unknown [$m/z=299.1$], 13. methyl stearate, 14. ethyl linoleate, 15. unknown [$m/z=313.3$], 16. docosane, 17. campesterol, 18. stigmasterol, 19. β -sitosterol.

1.7. GC-MS chromatograms of AI

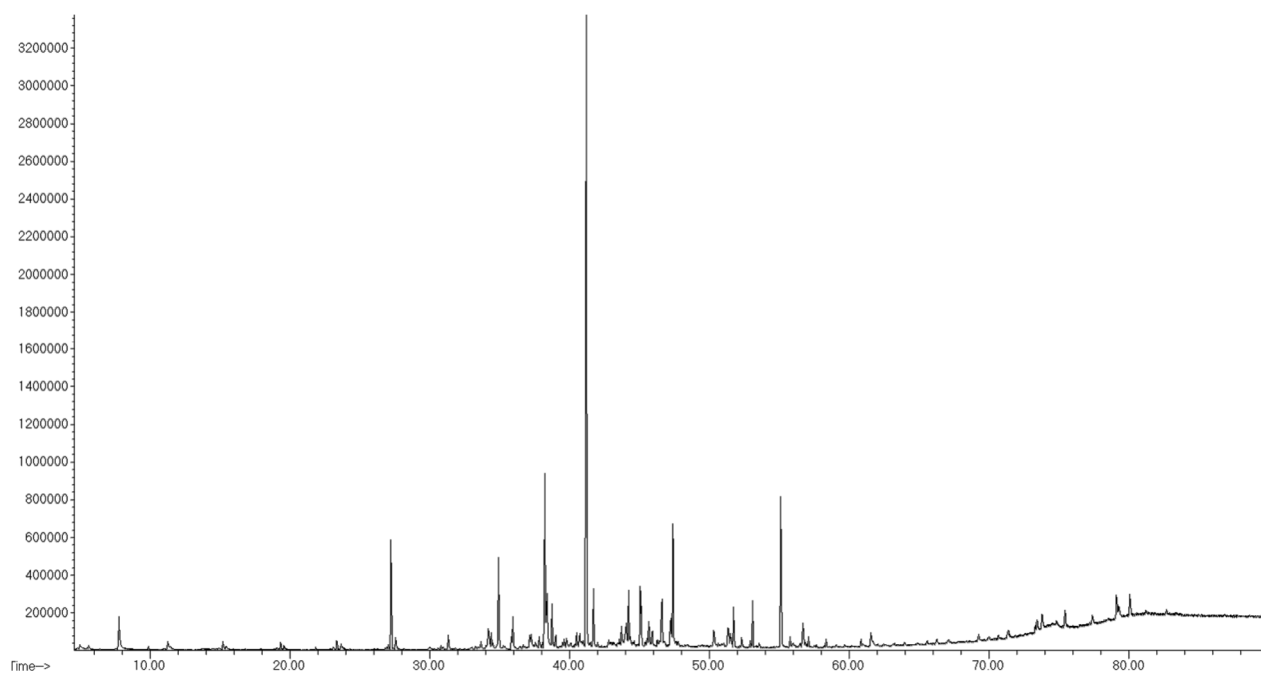


Figure S13. Total GC-MS chromatogram of AI.

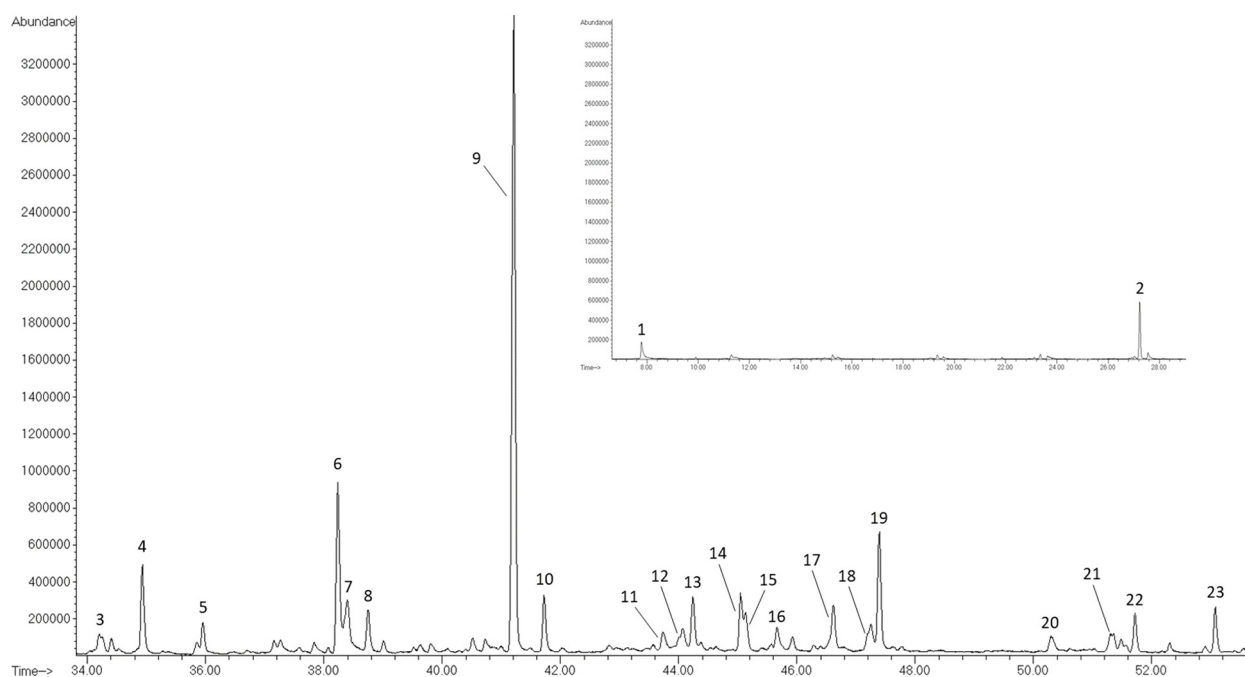


Figure S14. Zoomed GC-MS chromatogram of AI in the region of identified compounds. 1. pelargonaldehyde, 2. hexadecane, 3. 3-hexadecanone, 4. palmitaldehyde, 5. hexahydrofarnesyl acetone, 6. *trans*-2-nonadecene, 7. unknown [$m/z=266.1$], 8. methyl palmitate, 9. 2-octadecanone, 10. stearaldehyde, 11. stearyl alcohol, 12. methyl linoleate, 13. methyl oleate, 14. unknown [$m/z=282.1$], 15. methyl stearate, 16. oleic acid, 17. unknown [$m/z=283.3$], 18. ethyl stearate, 19. docosane, 20. tricosane, 21. methyl arachidate, 22. unknown [$m/z=323.3$], 23. tetracosane.

1.8. GC-MS chromatograms of AD_B

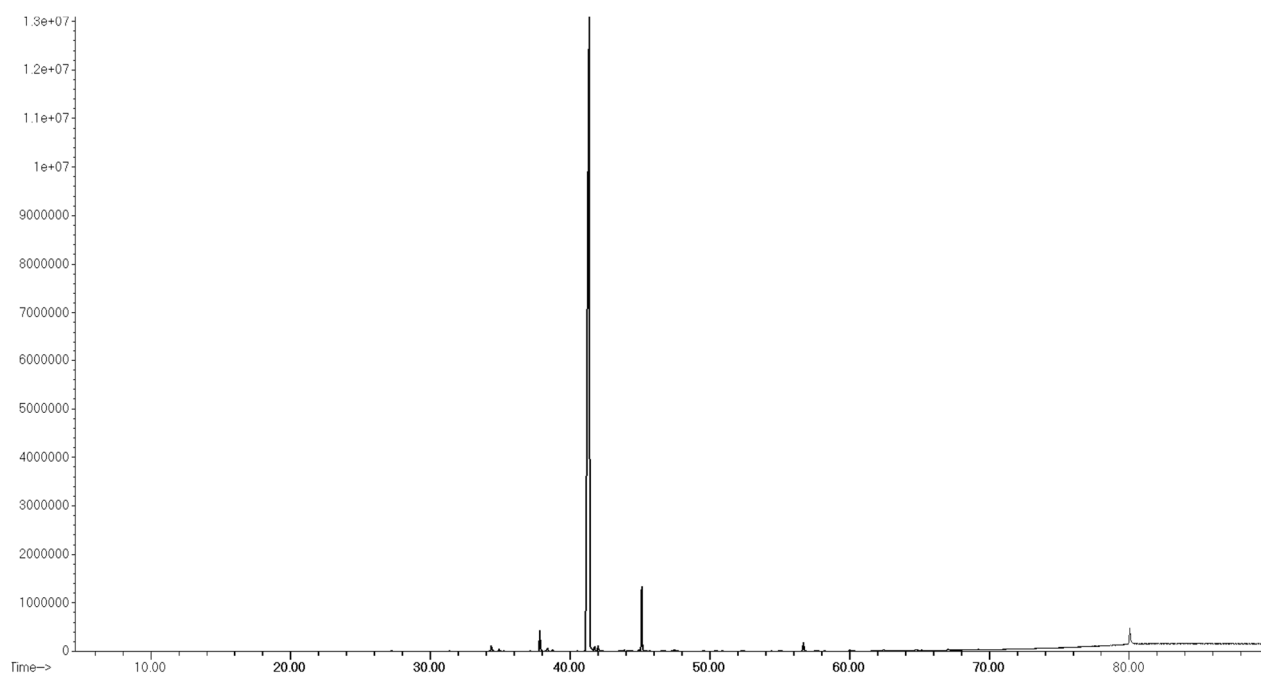


Figure S15. Total GC-MS chromatogram of AD_B.

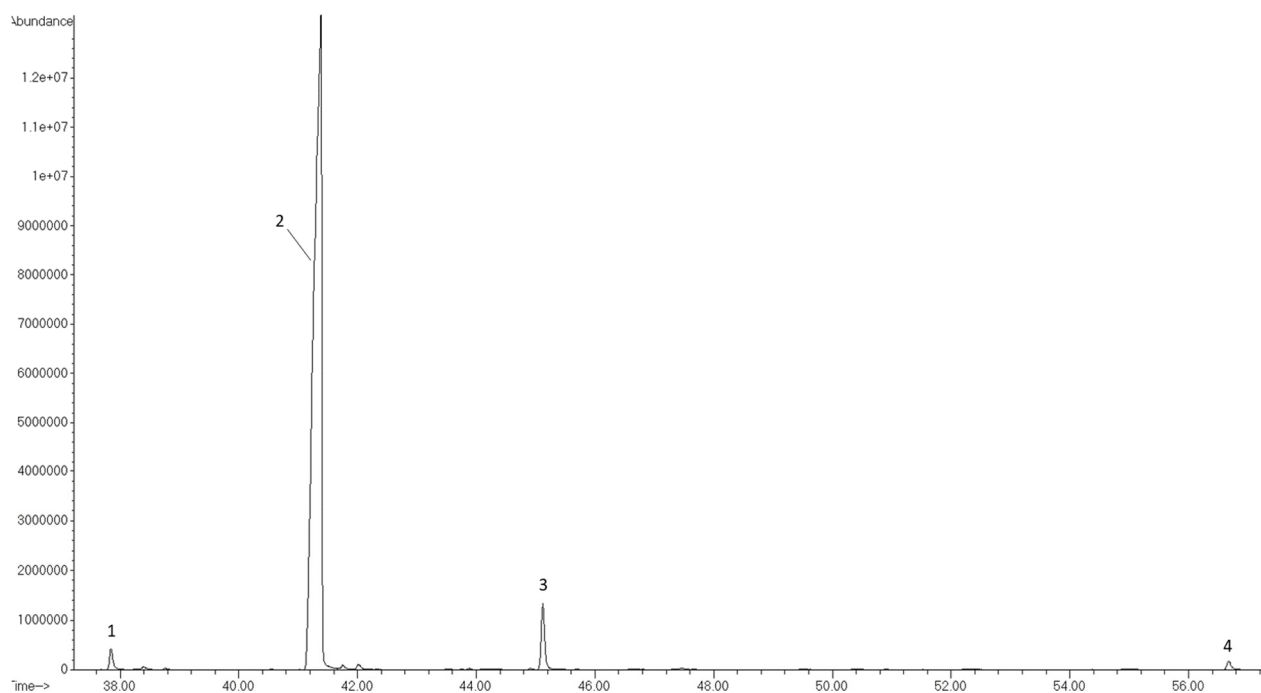


Figure S16. Zoomed GC-MS chromatogram of AD_B in the region of identified compounds. 1. 2-heptadecanone, 2. 2-octadecanone, 3. methyl stearate, 4. bis(2-ethylhexyl) phthalate.

1.9. GC-MS chromatograms of AF_A

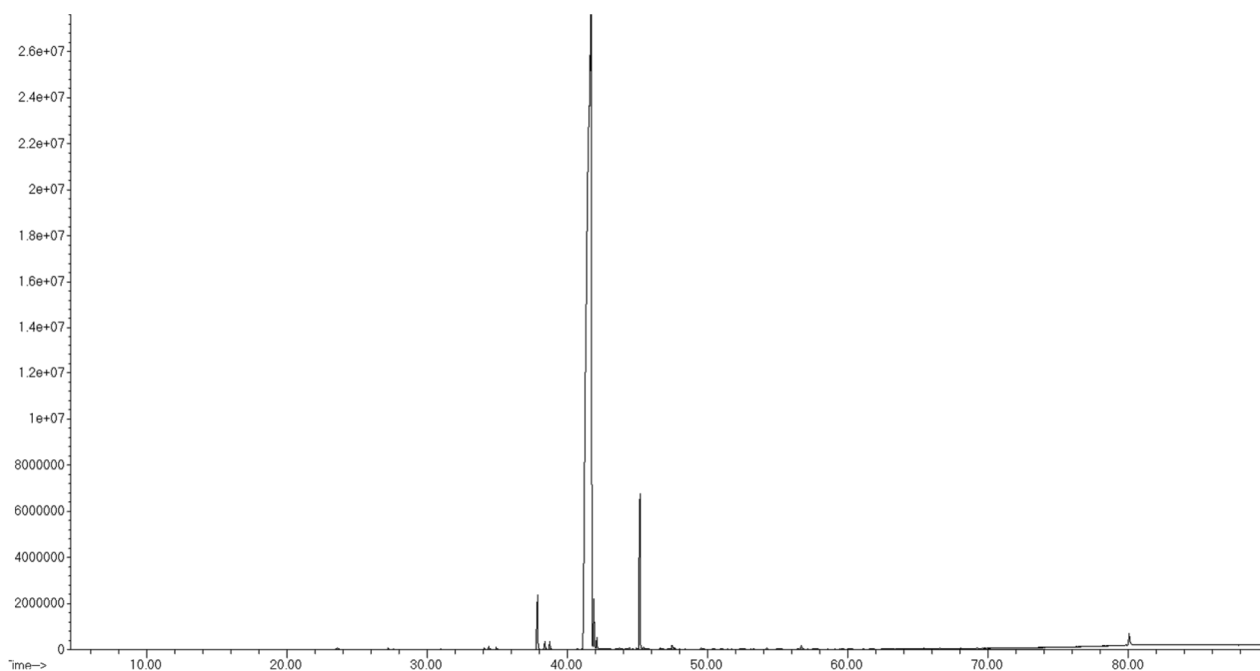


Figure S17. Total GC-MS chromatogram of AF_A.

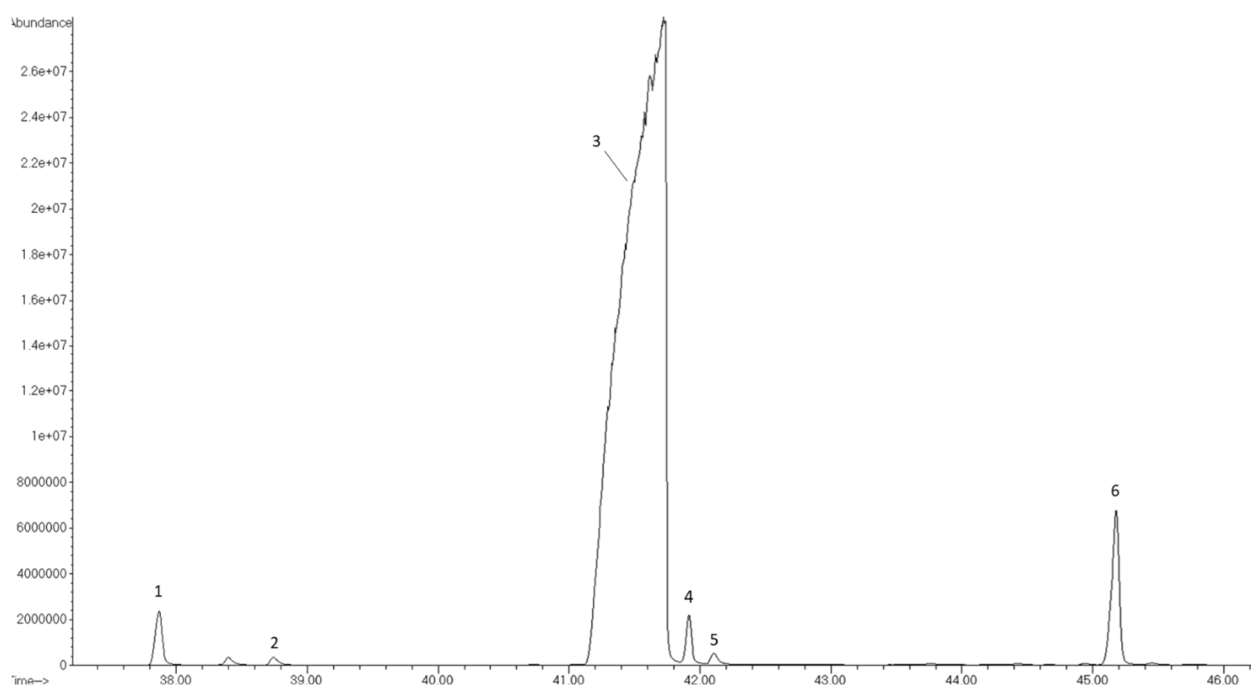


Figure S18. Zoomed GC-MS chromatogram of AF_A in the region of identified compounds. 1. 2-heptadecanone, 2. methyl palmitate, 3. 2-octadecanone, 4. stearaldehyde, 5. methyl margarate, 6. methyl stearate.

2. Spectra of the known compounds 1-5 and A3

2.1. Spectra of compounds 1 and 2

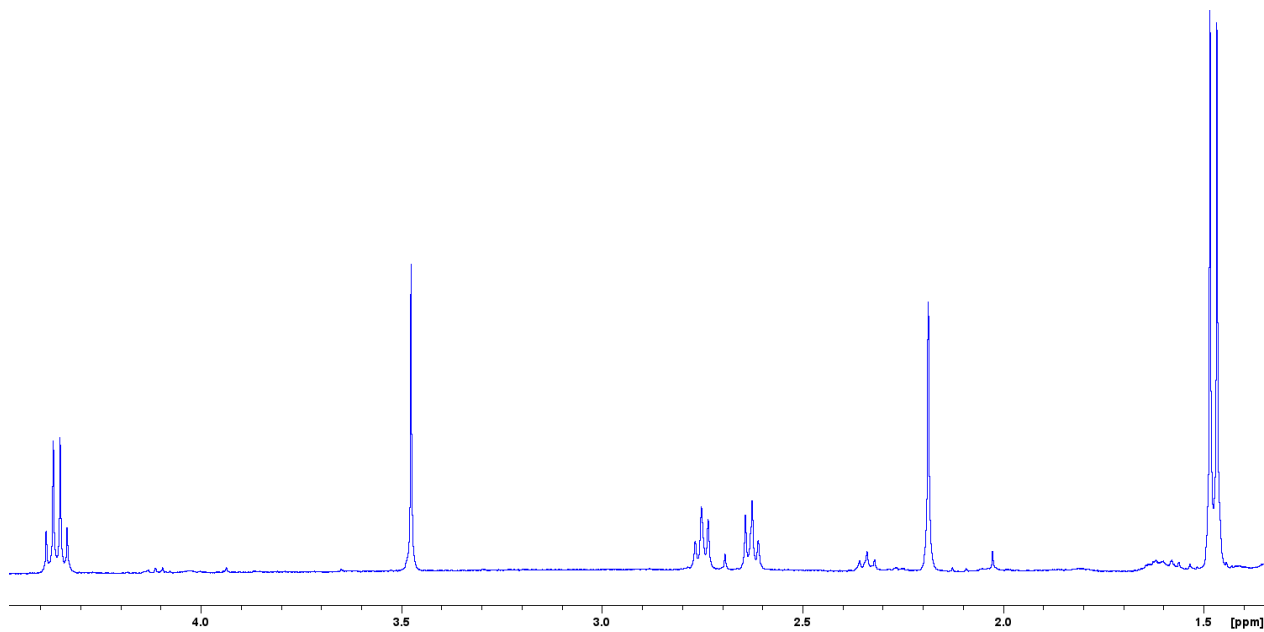


Figure S19. ^1H NMR (400 MHz, CDCl_3) spectrum of compounds 1 and 2.

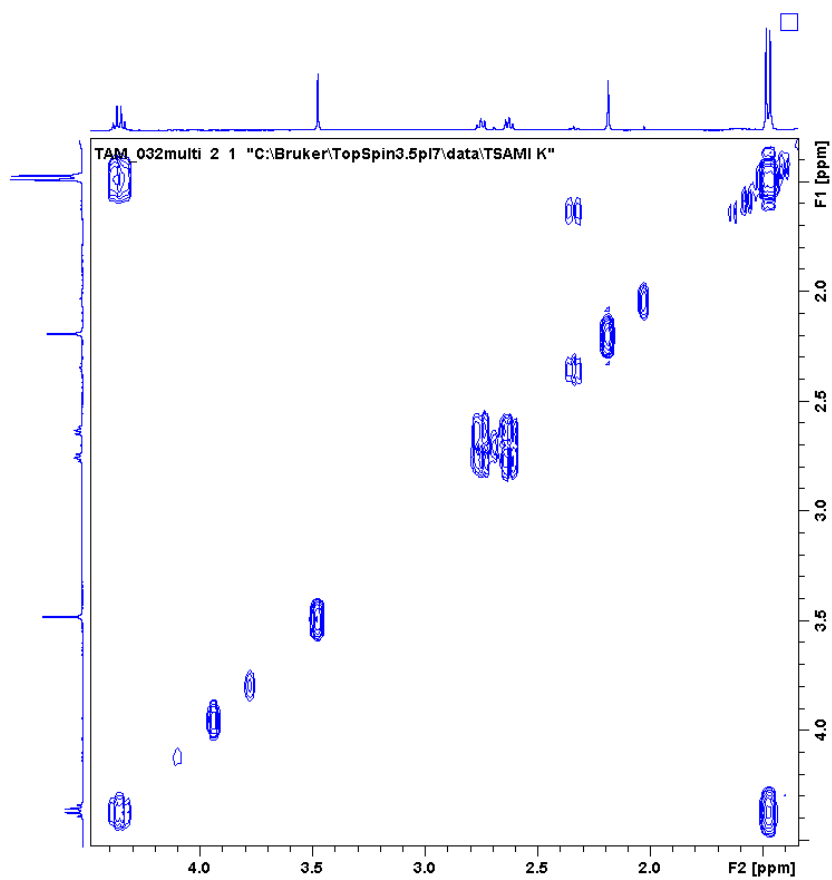


Figure S20. ^1H - ^1H COSY (CDCl_3) spectrum of compounds 1 and 2.

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2.3. Spectra of compound 4

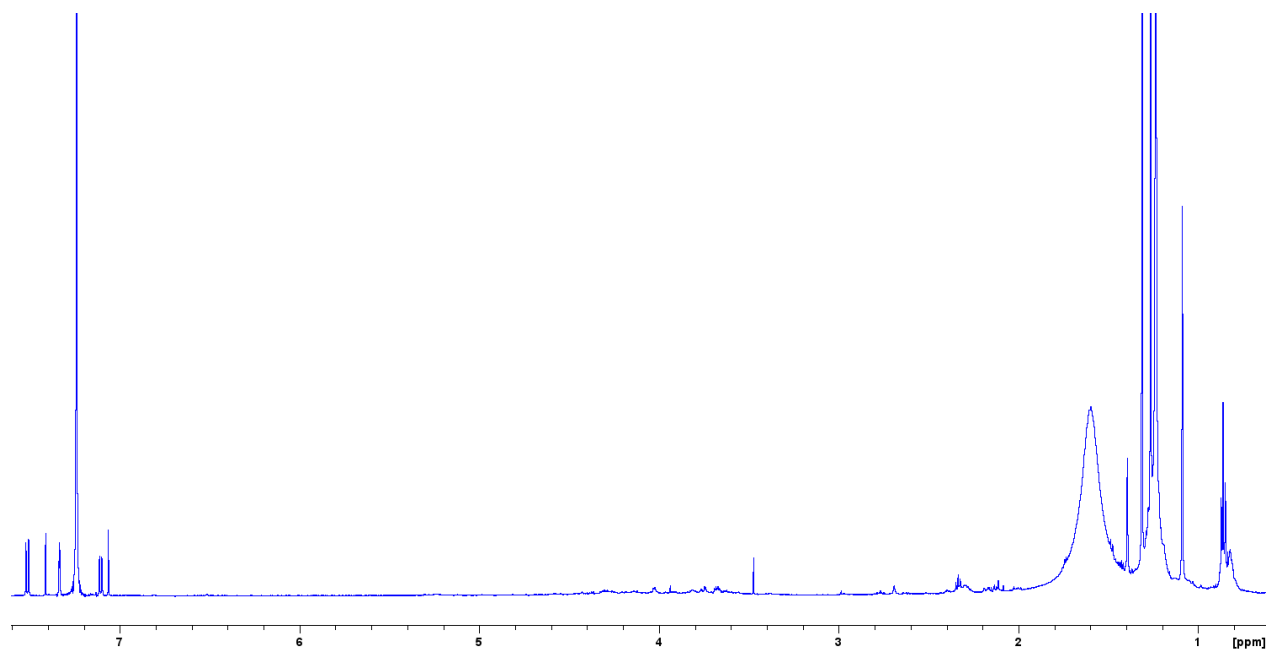


Figure S23. ^1H NMR (600 MHz, CDCl_3) spectrum of compound 4.

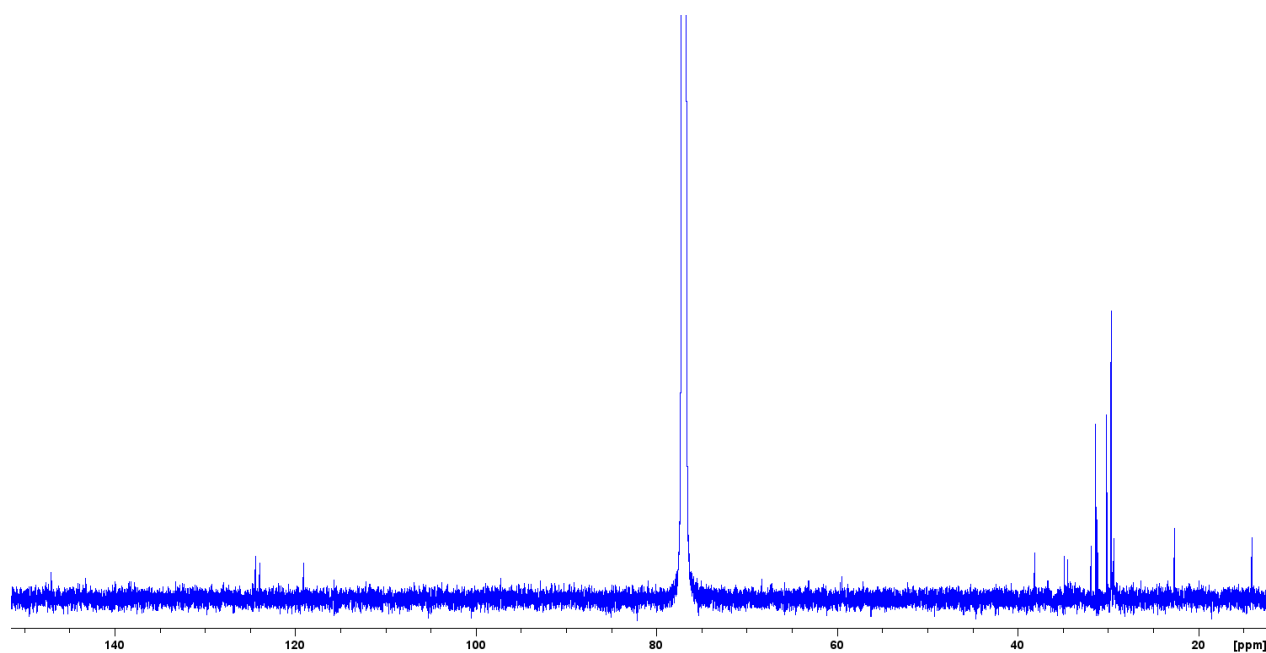


Figure S24. ^{13}C (150 MHz, CDCl_3) spectrum of compound 4.

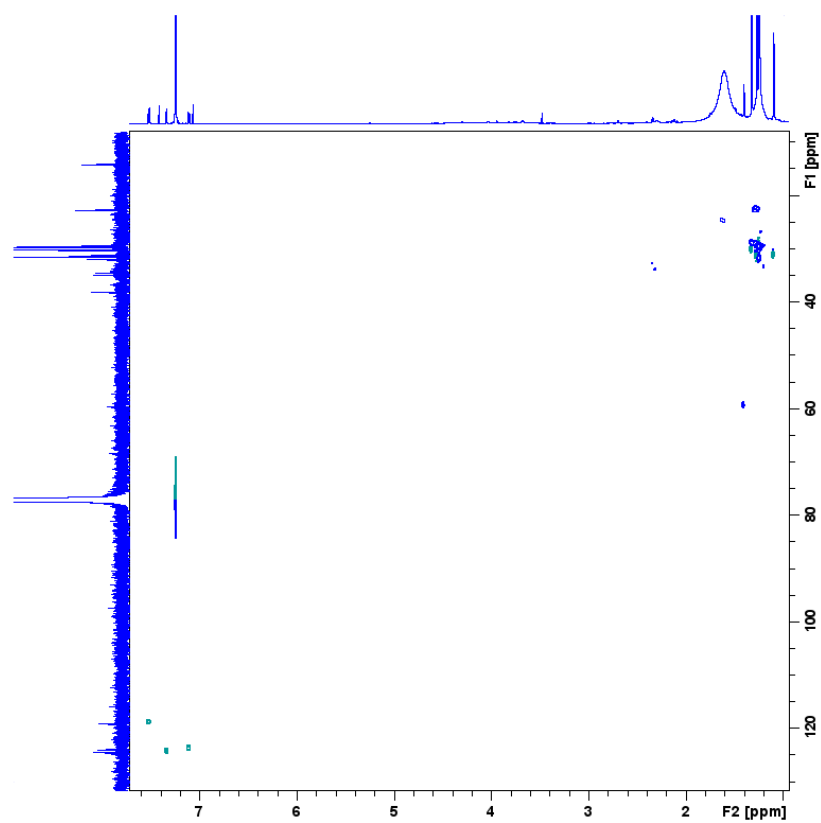


Figure S25. HSQC (CDCl₃) spectrum of compound **4**.

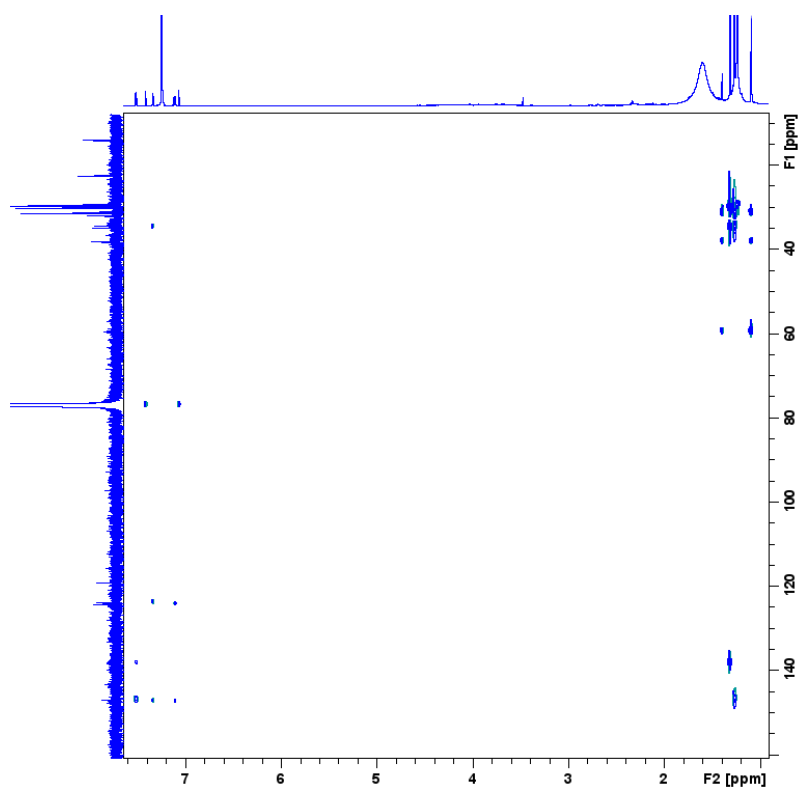


Figure S26. HMBC (CDCl₃) spectrum of compound **4**.

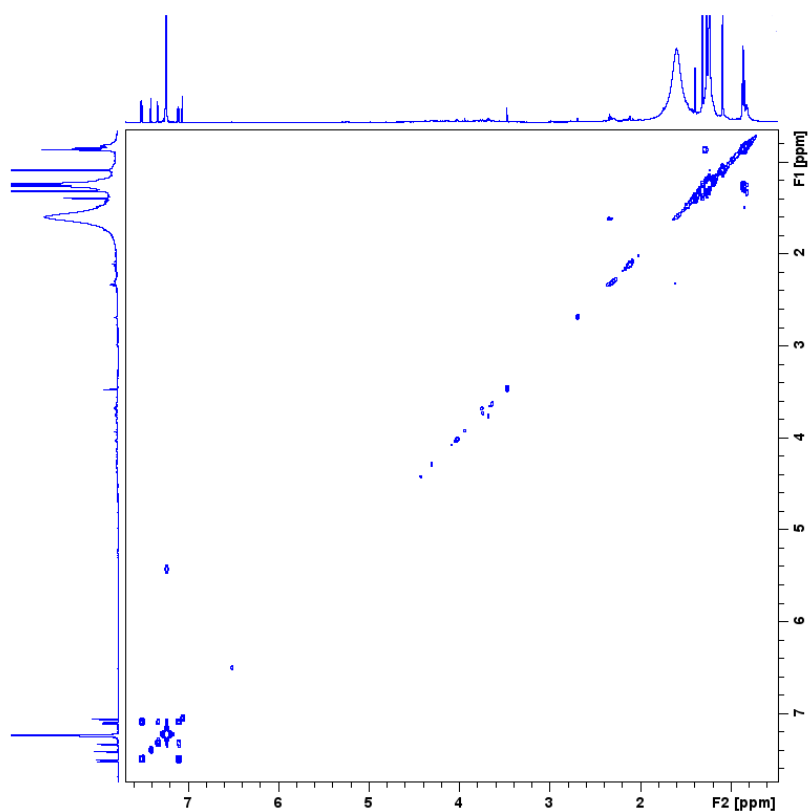


Figure S27. ^1H - ^1H COSY (CDCl_3) spectrum of compound **4**.

2.4. Spectra of compound **5**

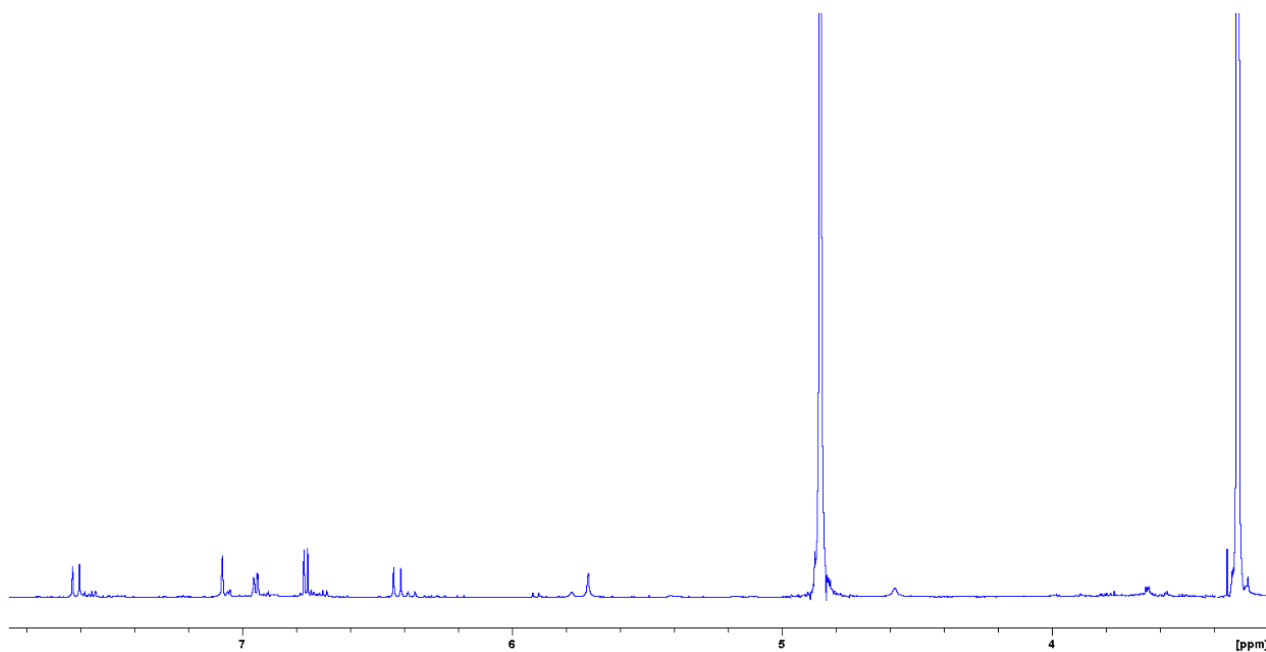


Figure S28. ^1H NMR (600 MHz, CD_4O) spectrum of compound **5**.

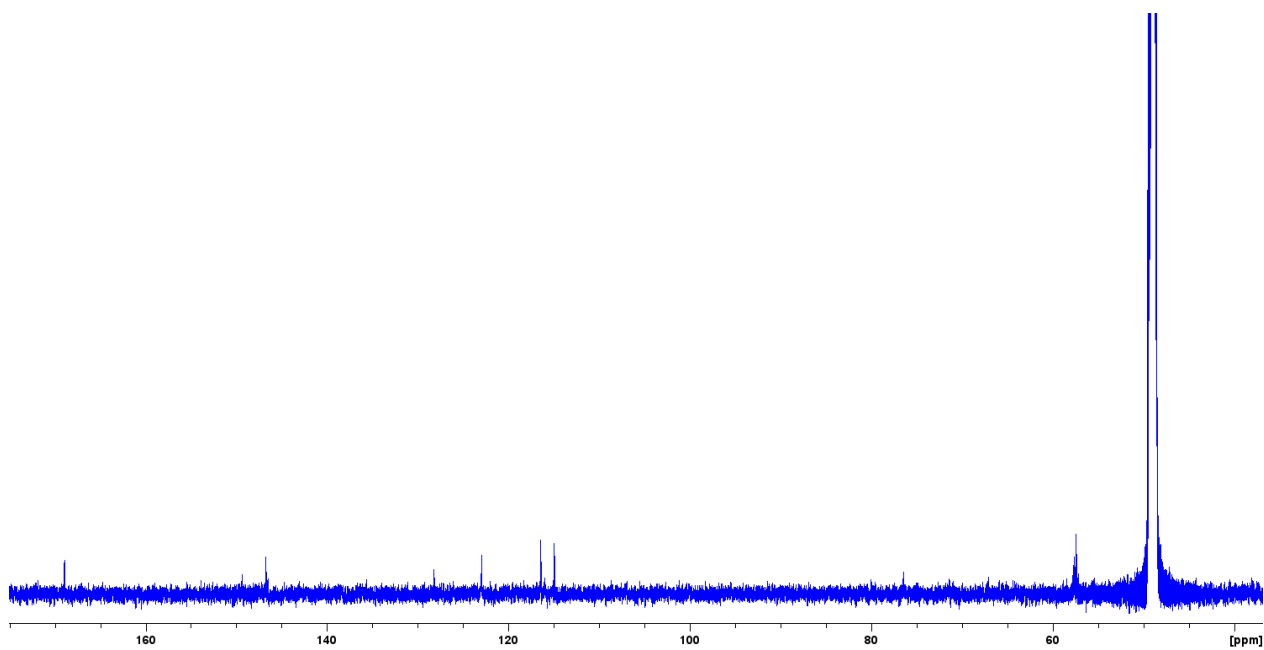


Figure S29. ^{13}C (150 MHz, CD_4O) spectrum of compound **5**.

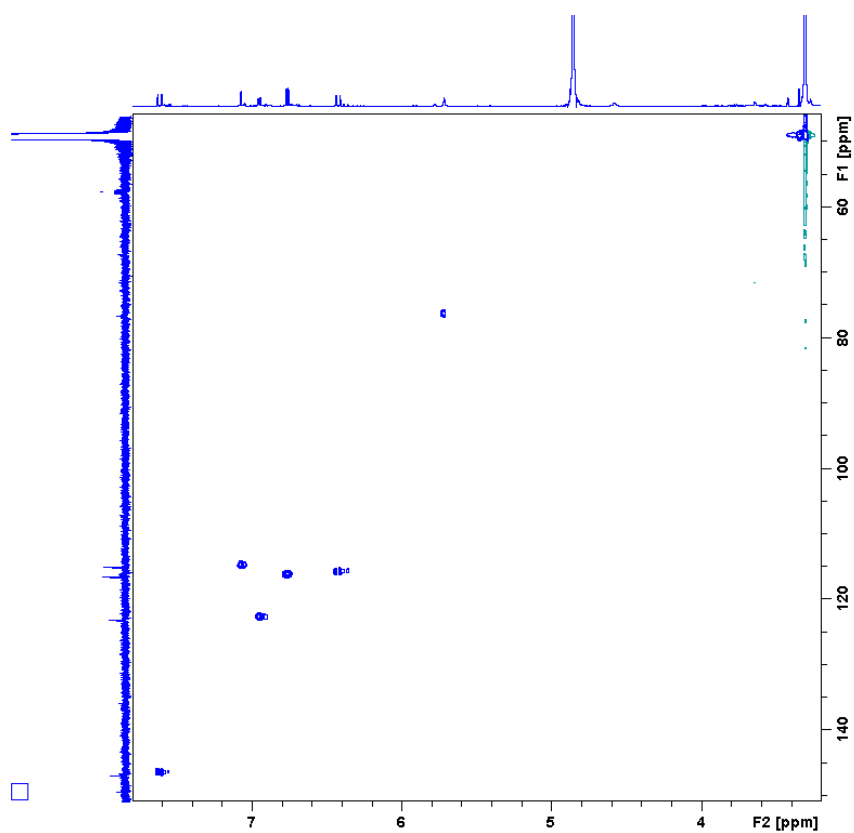


Figure S30. HSQC (CD_4O) spectrum of compound **5**.

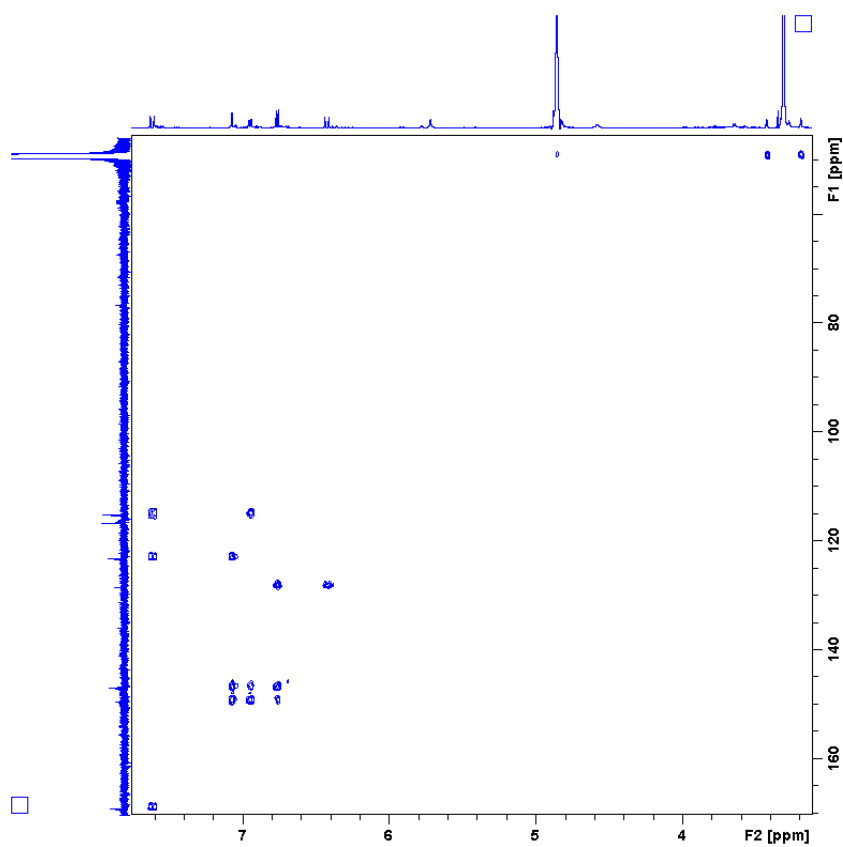


Figure S31. HMBC (CD₄O) spectrum of compound **5**.

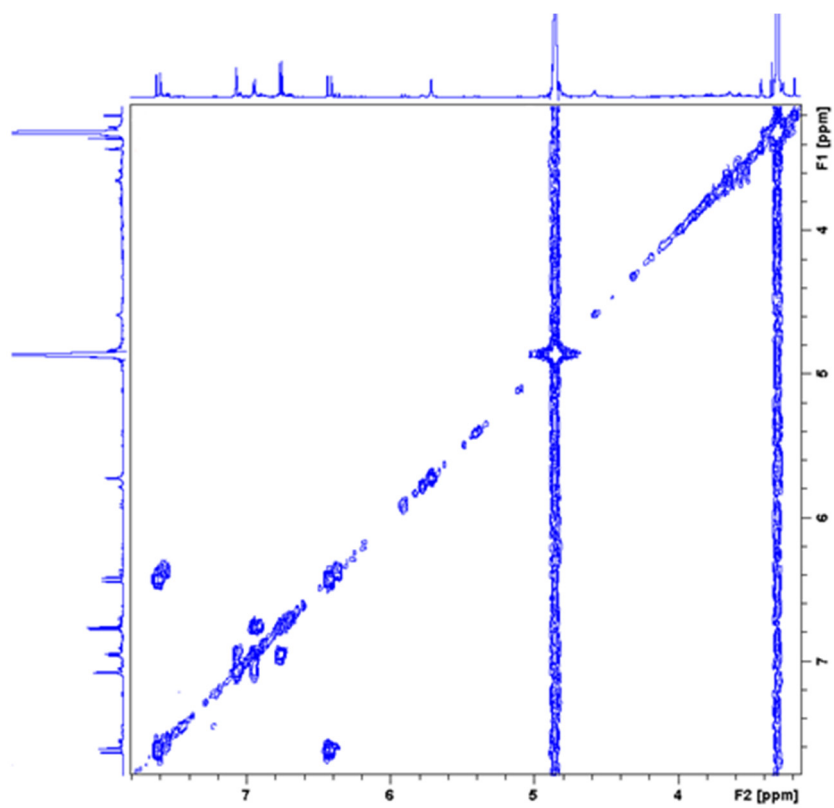


Figure S32. ¹H-¹H COSY (CD₄O) spectrum of compound **5**.

2.5. Spectrum of n-butanol extract (A3)

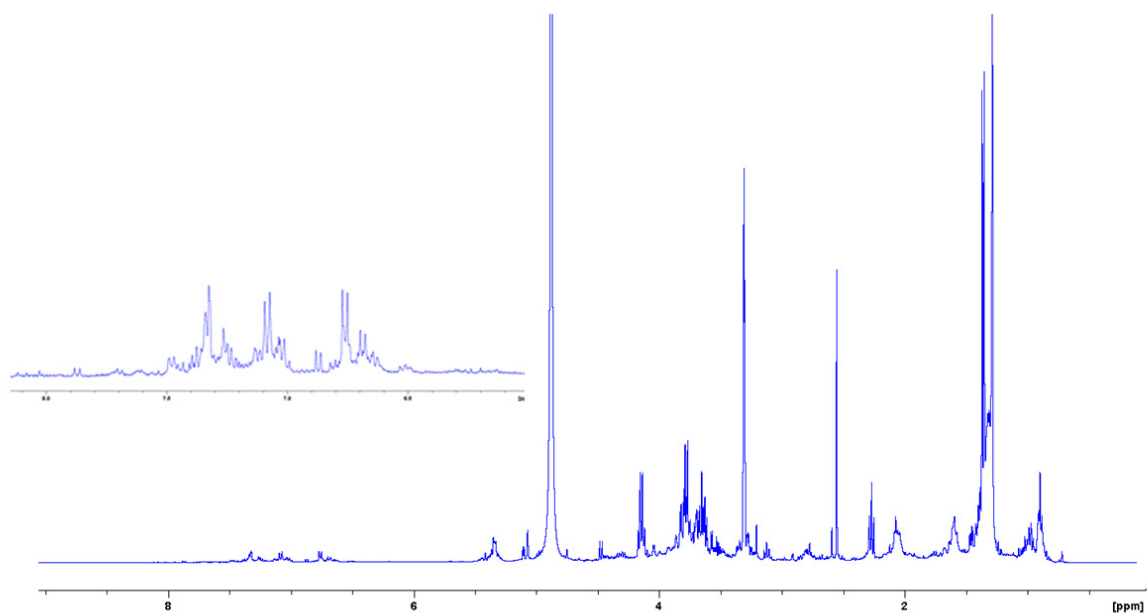


Figure S33. ^1H NMR (600 MHz, CD_4O) spectrum of n-butanol extract (A3).

3. LC-MS chromatograms of n-butanol extract (A3) in positive ion mode

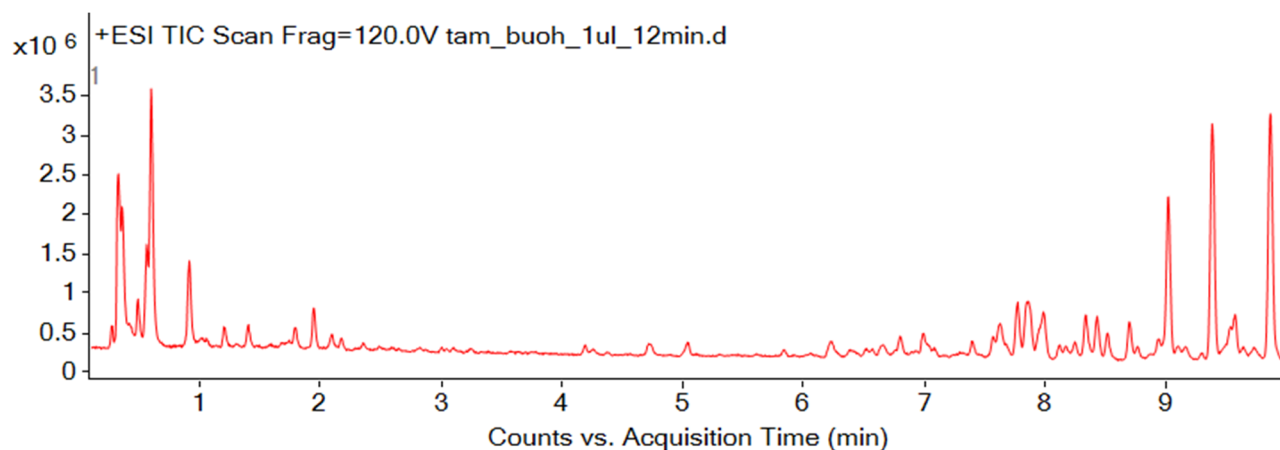


Figure S34. TIC of BuOH extract in positive ion mode.

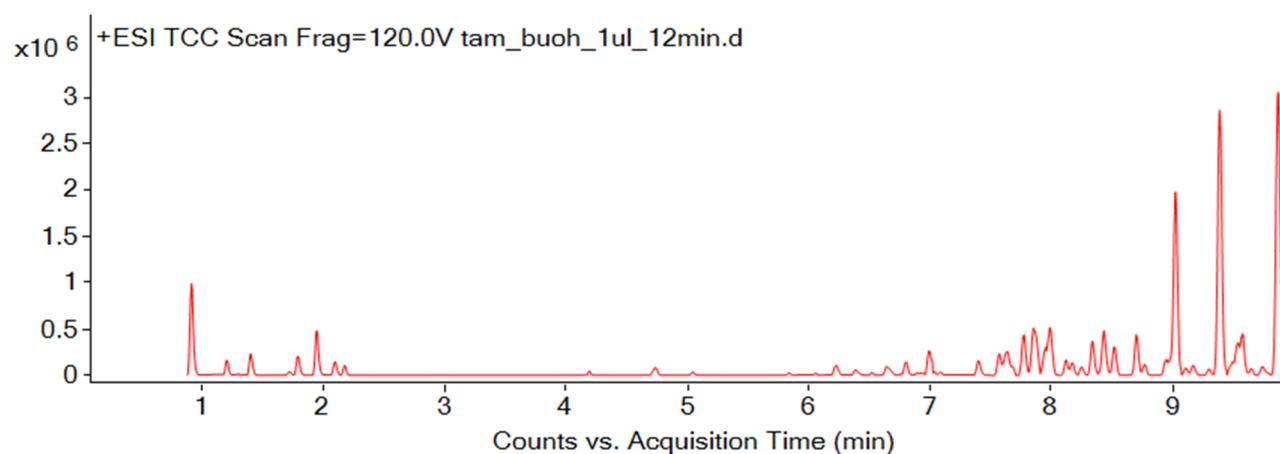


Figure S35. TCC of BuOH extract in positive ion mode.

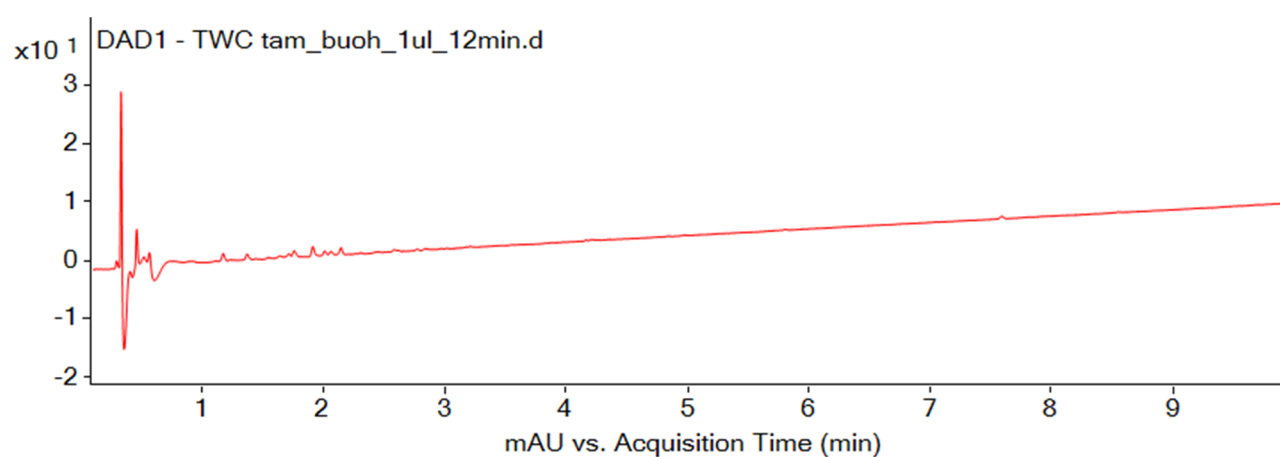


Figure S36. UV of BuOH extract in positive ion mode.

4. LC-MS chromatograms of n-butanol extract (A3) in negative ion mode

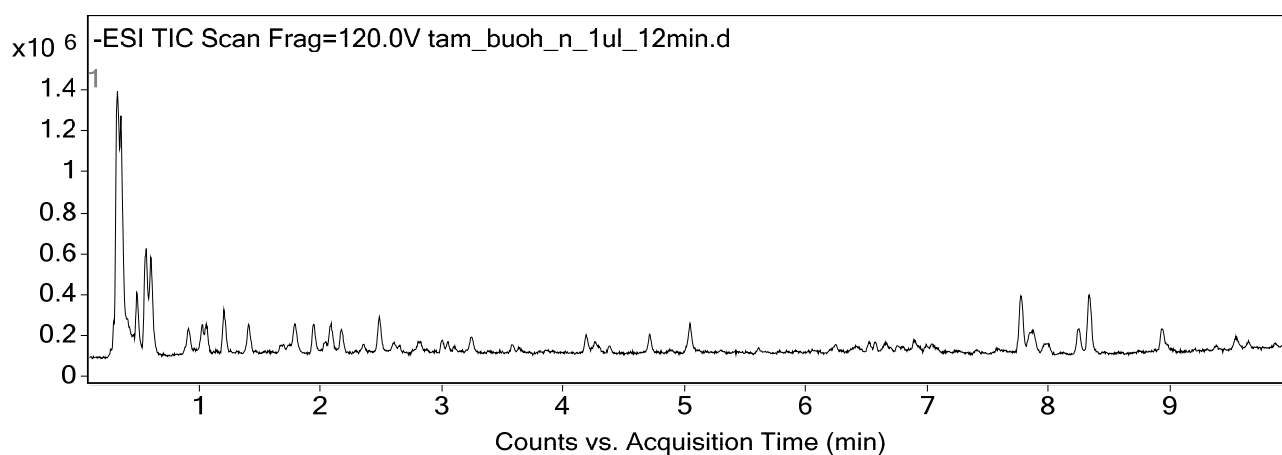


Figure S37. TIC of BuOH extract in negative ion mode.

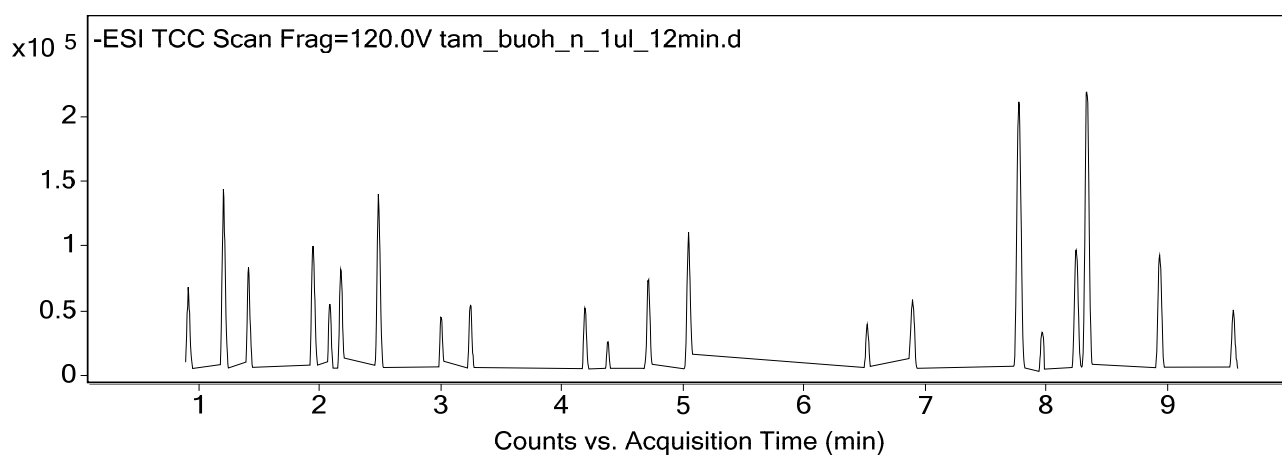


Figure S38. TCC of BuOH extract in negative ion mode.

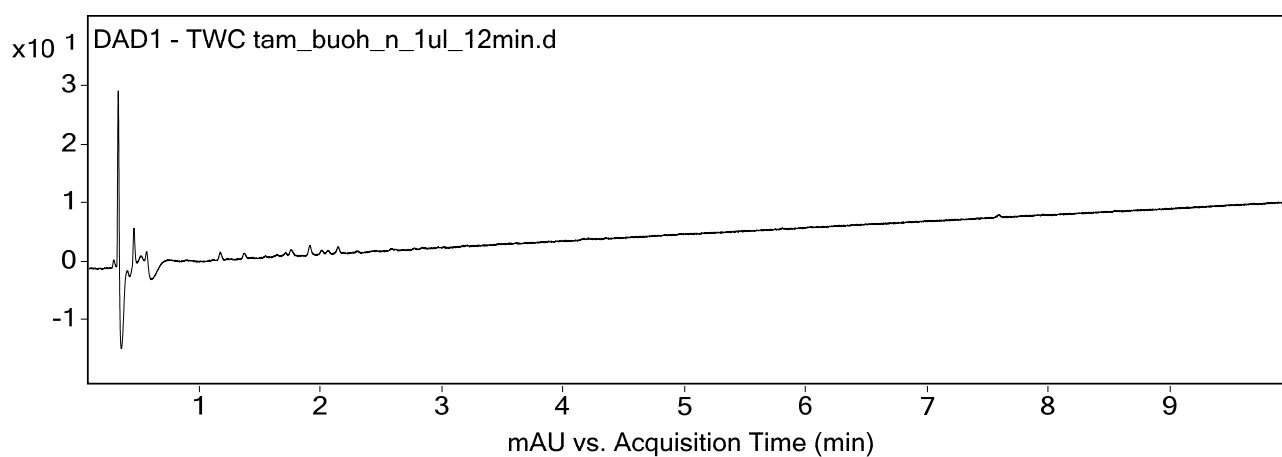
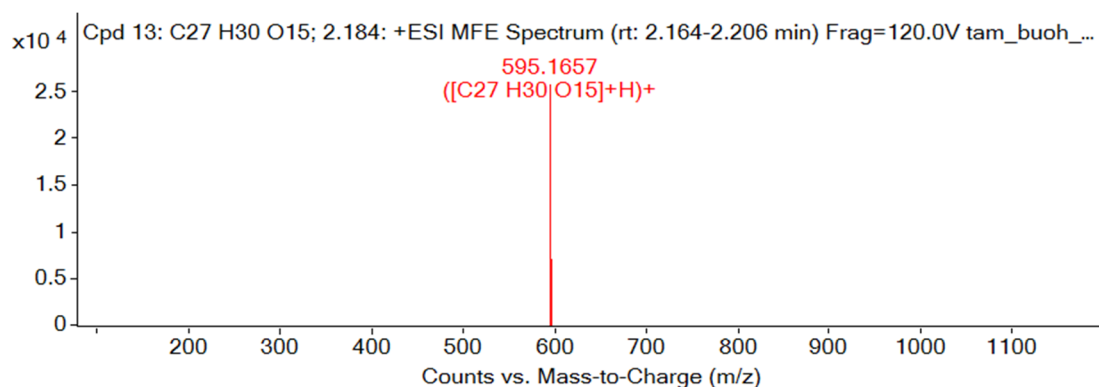
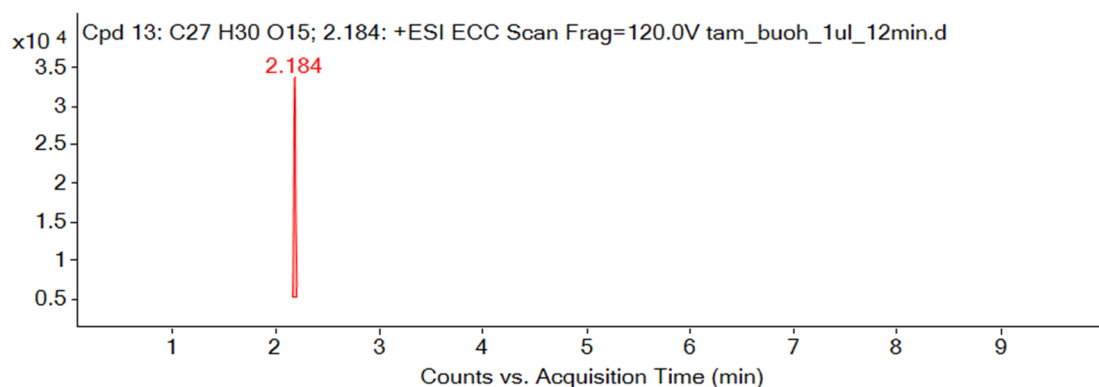


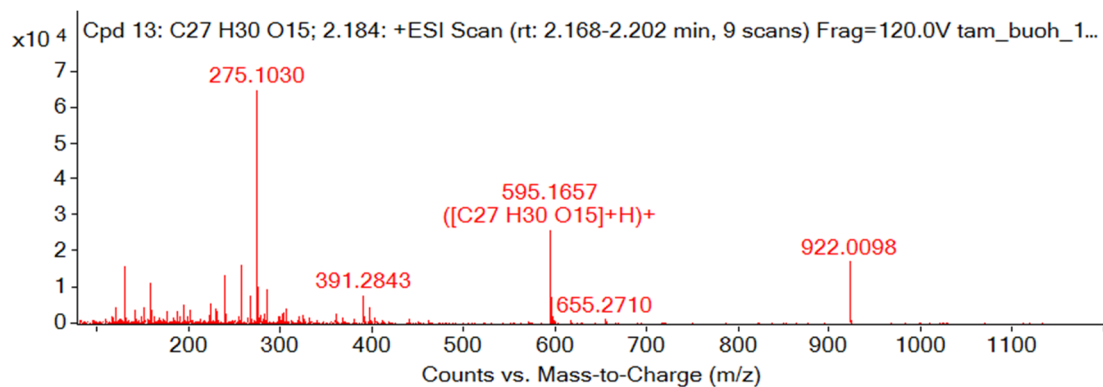
Figure S39. UV of BuOH extract in negative ion mode.

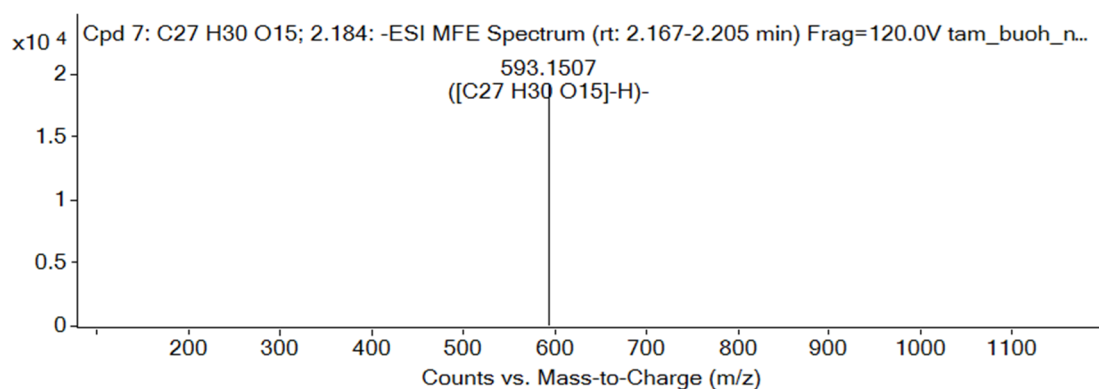
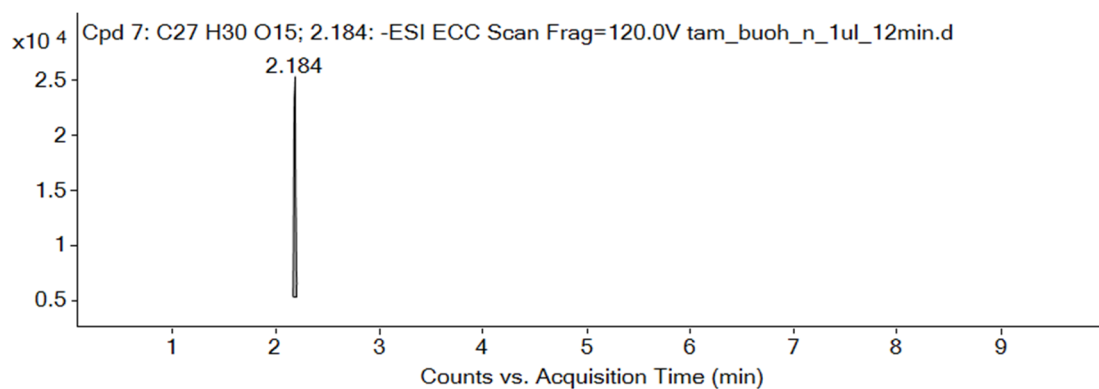
5. LC-MS data of kaempferol 3-*O*-rutinoside and hydroxy-3-methoxyphenyl)heptane in positive and negative ion mode



Peak List

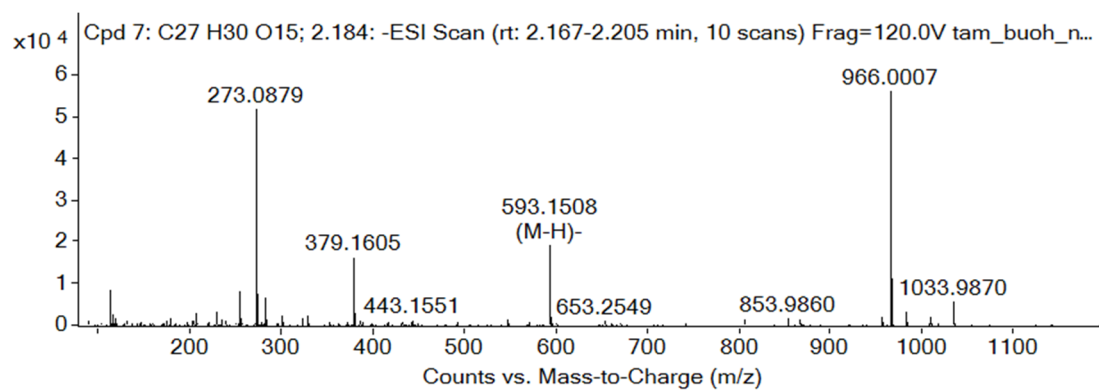
<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
595.1657	1	25771.34	C ₂₇ H ₃₀ O ₁₅	[M+H] ⁺
596.169	1	7080.18	C ₂₇ H ₃₀ O ₁₅	[M+H] ⁺

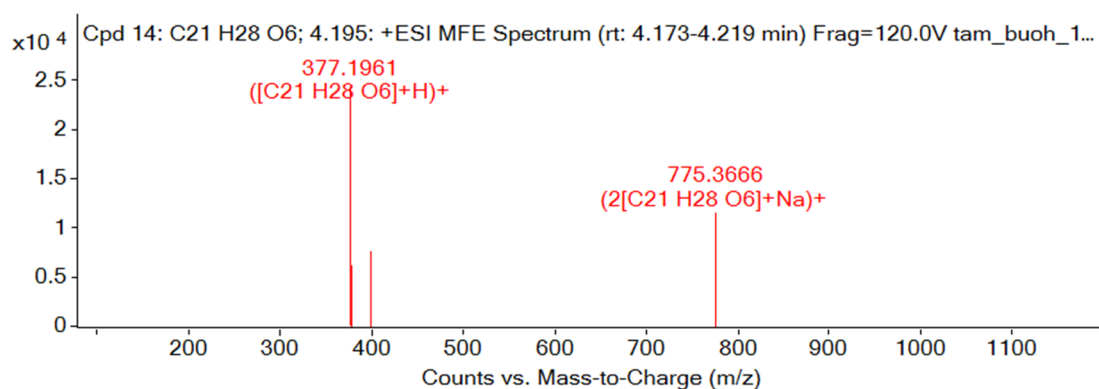
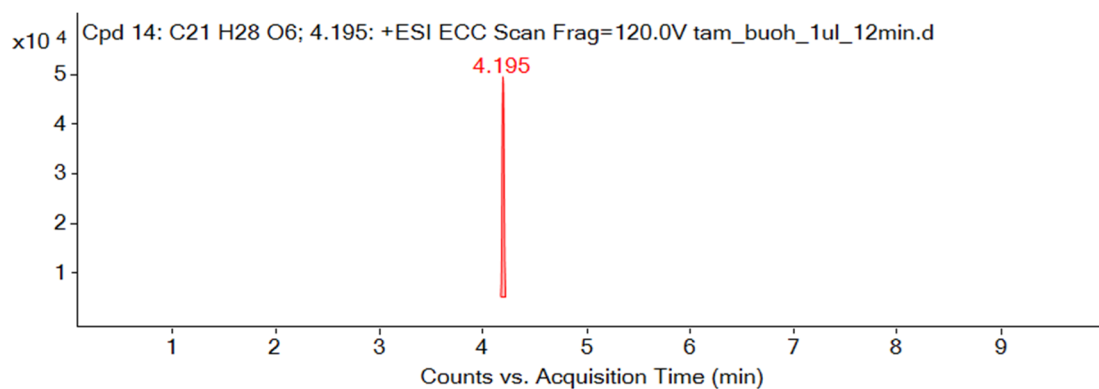




Peak List

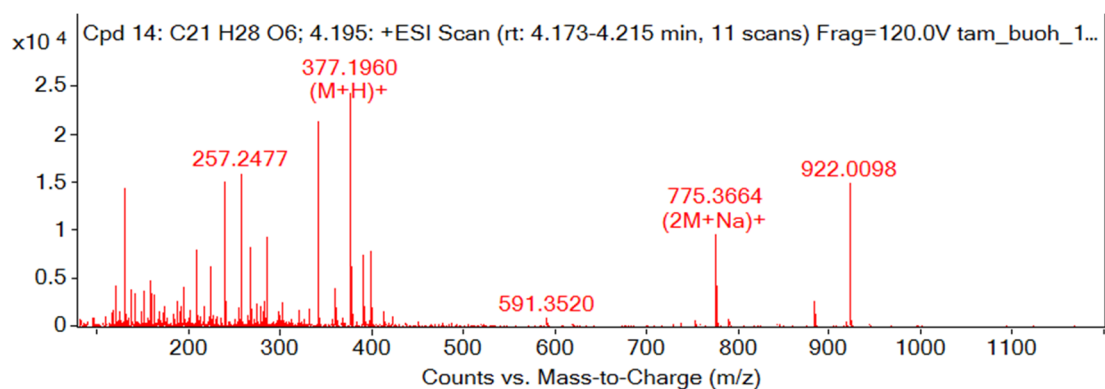
<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
593.1507	-1	19189.44	C ₂₇ H ₃₀ O ₁₅	(M-H) ⁻
594.1541	-1	6397.60	C ₂₇ H ₃₀ O ₁₅	(M-H) ⁻

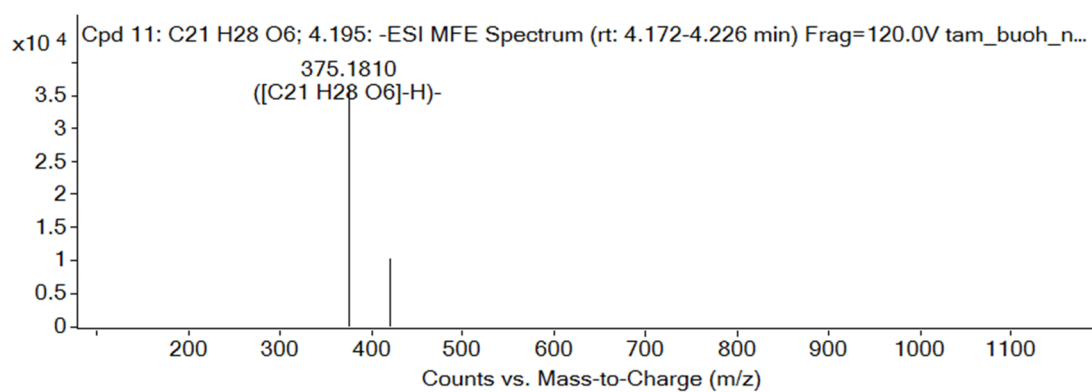
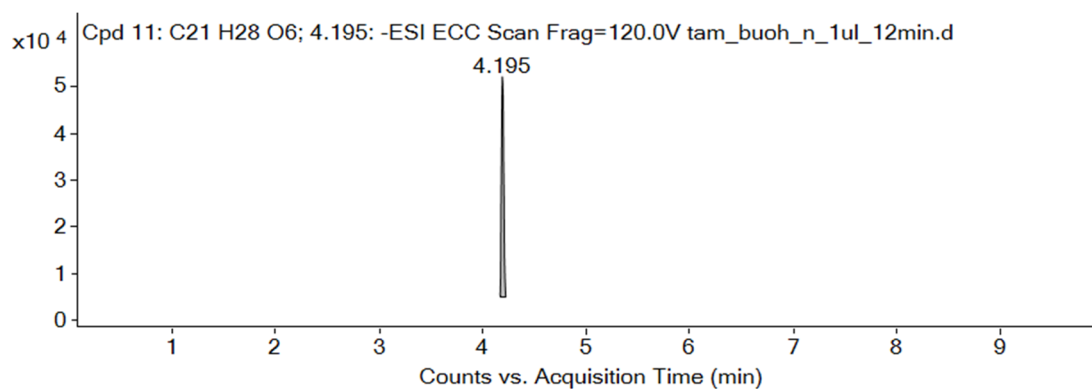




Peak List

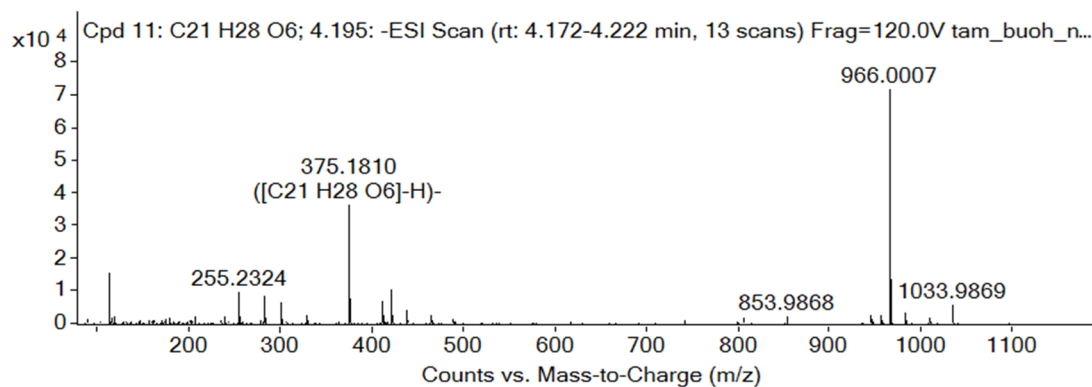
<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
593.1507	-1	19189.44	C ₂₇ H ₃₀ O ₁₅	(M-H) ⁻
594.1541	-1	6397.60	C ₂₇ H ₃₀ O ₁₅	(M-H) ⁻





Peak List

m/z	z	Abund	Formula	Ion
375.181	-1	36080.38	C ₂₁ H ₂₈ O ₆	(M-H) ⁻
376.1844	-1	7622.61	C ₂₁ H ₂₈ O ₆	(M-H) ⁻
421.1861	-1	10404.67	C ₂₁ H ₂₈ O ₆	(M+HCOO) ⁻



6. Flow chart of the isolation procedures

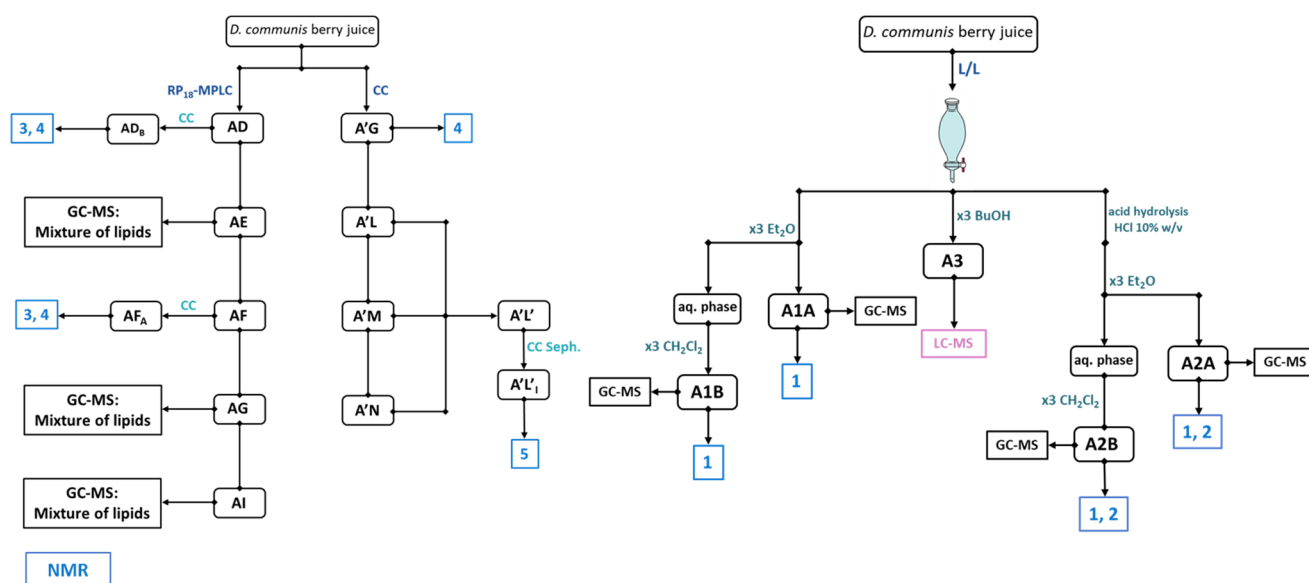


Figure S40. Flow chart of the isolation procedures of *D. communis* berry juice (MPLC, CC, GC-MS, LC-MC and NMR).

7. GC-MS tables of AD_B and AF_A

Table S1. Chemical composition of fraction AD_B

No.	Retention time	% Area	KI	AI	Name of compound	Molecular formula	MW
1	37.850	1.3	1897	1901	2-heptadecanone	C ₁₇ H ₃₄ O	254
2	41.380	93.8	2005	2004	2-octadecanone	C ₁₈ H ₃₆ O	268
3	45.126	4.2	2125	2124	octadecanoic acid, methyl ester [methyl stearate]	C ₁₉ H ₃₈ O ₂	298
4	56.680	0.7		2550	1,2-benzenedicarboxylic acid, bis(2-ethylhexyl) ester [bis(2-ethylhexyl) phthalate]	C ₂₄ H ₃₈ O ₄	390
Total		100					

Table S2. Chemical composition of fraction AF_A

No.	Retention time	% Area	KI	AI	Name of compound	Molecular formula	MW
1	37.870	1.31	1898	1901	2-heptadecanone	C ₁₇ H ₃₄ O	254
2	38.745	0.22	1924	1921	methyl palmitate [hexadecanoic acid, methyl ester]	C ₁₇ H ₃₄ O ₂	270
3	41.723	93.08	2016	2004	2-octadecanone	C ₁₈ H ₃₆ O	268
4	41.916	0.98	2022	2021	octadecanal	C ₁₈ H ₃₆ O	268

5	42.110	0.28	2028	2028	heptadecanoic acid, methyl ester	$C_{18}H_{38}O_2$	284
6	45.181	4.13	2127	2124	methyl stearate	$C_{19}H_{38}O_2$	298
Total		100					

Components are listed in all Tables according to their elution from a HP-5MS column. KI: Kováts indices calculated against C_9 - C_{25} n-alkanes on the HP-5MS column; AI: arithmetic indices; tr: traces.